Wave Invariants on Flat Tori

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Dipl.-Math. Tillmann Berg

Präsidentin der Humboldt-Universität zu Berlin
Prof. Dr. Sabine Kunst

Dekan der Mathematisch-Naturwissenschaftlichen Fakultät
Prof. Dr. Elmar Kulke

Gutachter/innen:	Prof. Dr. Dorothee Schüth
	Prof. Dr. Christian Bär
	Prof. Dr. Olaf Post
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HUMBOLDT-UNIVERSITÄT ZU BERLIN

TillmannBerg@gmx.de

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Abstract

This thesis is concerned with Schrödinger operators acting on the sections of a Hermitian line bundle over an even-dimensional flat torus. Schrödinger operators are constructed from a connection on the bundle and a potential, a function on the torus. Restricting to *translation-invariant* connections and line bundles with *nondegenerate* Chern class we study the extent to which the spectrum of the Schrödinger operator of a given potential determines the connection.

Negative spectral results, i.e. differences in connections not determined by spectra, are obtained by constructing *transplantations*. To obtain positive results we compute the first five *wave invariants* of the Schrödinger operators explicitly using the computer algebra software MATHEMATICA. For simple potentials we find a full characterization of the isospectrality of the translation-invariant connections.

We also prove general properties of the wave invariants, which imply a more general existence of nonisospectral connections but which also show limitations of the spectral information contained within finitely many wave invariants.

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Introduction

Let M be an n-dimensional *flat torus* $\mathbb{R}^n/\mathcal{L}$ given by some *lattice* $\mathcal{L}$. Every *potential* $Q \in C^\infty(M)$ can be interpreted as a smooth $\mathcal{L}$-periodic function $Q\colon \mathbb{R}^n \to \mathbb{R}$. It gives rise to a Schrödinger operator $\Delta + Q$ on $\mathbb{R}^n$. It has been extensively studied, for example in [ERT84a] and [ERT84b], whether the potential is determined by the spectrum of the *Schrödinger operator* acting on periodic functions or on functions satisfying $f(x+l) = \mathrm{e}^{2\pi \mathrm{i} a(l)} f(x)$ for all $l \in \mathcal{L}$ for some $a \in \mathbb{R}^{n\prime}$. In [Gui90] Victor Guillemin showed that the spectrum of the Schrödinger operator arising from a *connection* ∇ on a given Hermitian *line bundle* λ over M determines the potential if a number of assumptions is satisfied.

In [GGKW08] Carolyn S. Gordon, Pierre Guerini, Thomas Kappeler and David L. Webb computed the first wave invariant and parts of the second wave invariant of the Schrödinger operator of a connection acting on the sections of a line bundle and used these to show that parts of the potential are spectrally determined under certain conditions. It was assumed that the curvature of each connection is both translation-invariant and nondegenerate. A connection is translation-invariant if its curvature is given by a constant antisymmetric 2-form $-2\pi F$ on $\mathbb{R}^n$. The nondegeneracy requires the torus to be even-dimensional and it also gives a normal form for the Hermitian line bundle described by Chern invariant factors $r_1 | \cdots | r_{n/2}$.

If all these integers are one, it was shown in [GGKW08] that the potential Q is spectrally determined by the collection of all spectra given by all such connections. If a single connection is weakly $\mathbb{Z}_2$-invariant then the even part of the potential is determined by the corresponding (single) spectrum.

In this thesis we will stay within the general setting of [GGKW08] but we will not assume that all Chern invariant factors are one. We will study the inverse question: Given a potential Q to what extent is the connection determined by the spectrum of its Schrödinger operator?

In Chapter 1 we will give a more detailed description of the line bundles, Laplacians and their spectra. In particular, we recall why it is sufficient to consider only translation-invariant connections given by $\nabla^{\mathrm{D}} + a$ for some *distinguished connection* ∇^{D} and 1-form $a \in \mathbb{R}^{n\prime}$.

In Chapter 2 we will construct new, explicit *transplantations* to show that two connections $a, b \in \mathbb{R}^{n\prime}$ are isospectral if the triple (Q, a, b) is of certain types, called (P) or (M). With the Laplace operator Δ_a^{D} induced by $\nabla^{\mathrm{D}} + a$ we show the following Theorem.

Theorem 2.14. If Q is a smooth potential on a flat torus M and two translation-invariant connections on a nondegenerate line bundle ω are given by $a, b \in \mathbb{R}^{n\prime}$ such that (Q, a, b) is of type (P) or of type (M) then $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b^{\mathrm{D}} + Q$ are isospectral,

$$\mathrm{Spec}_a(Q, \omega) = \mathrm{Spec}_b(Q, \omega)\,.$$

A well-known corollary of this Theorem is that all connections are isospectral if Q is constant.

To obtain positive results we will compute two types of spectral invariants: The *heat invariants* and the *wave invariants*.

We will first compute the much simpler heat invariants in Chapter 3, where we will follow [Gil95] for the general principle. However, instead of using functorial arguments we will compute the heat invariants directly. Although each step in those computations is elementary the size of intermediate expressions will increase very quickly with the index of the heat invariants, even for our flat manifold. Higher invariants are impossible to compute by hand and we give a MATHEMATICA notebook in Appendix C and digitally in [Ber18] that will enable us to compute the first 14 heat invariants, see Theorem 3.28. Apart from providing more invariants than [Gil95] (for our setting) this computation serves two more purposes: Firstly, it is a much simpler introduction to the computation of invariants using computer algebra software than the wave invariants. Secondly, we compute so-called "small" wave invariants $\mathsf{wi}_{k,d}(a, Q)$ in Chapter 5 for $d \in |\mathcal{L}|\backslash\{0\}$. The method used for this computation is only valid for $d \neq 0$ but we can use the heat invariants to show these expressions are spectral invariants for $d = 0$, as well.

The heat invariants do not contain the connection a and we have to compute other invariants if we want to obtain spectral information regarding the connection. The main focus of this thesis lies on the explicit computation of the first *five wave invariants* of the Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$. In Chapter 4 we will first follow [GGKW08] and sketch their approach to the wave trace and its asymptotic expansion. The existence of an approachable normal form of the nondegenerate line bundles ω over M allows us to give an explicit algorithm for the computation of the wave invariants given in Section 4.4, which is the point where we go beyond what has been done in [GGKW08].

It follows from this recipe that the wave invariants are of the form

$$\mathsf{WI}_{k,d}(a, Q) = \sum_{|l|=d} E_a(l) \cdot \sigma_l \cdot \mathsf{WI}_{k,l}(a, Q)\,,$$

where we sum over all lattice vectors l of equal, nonzero length d, where $E_a = \exp(-2\pi \mathrm{i} a)$ and σ_l is some signature. We call $\mathsf{WI}_{k,l}(a, Q)$ *partial wave invariant*. Instead of immediately giving a MATHEMATICA notebook for the

general computation of the wave invariants we will compute the first two invariants manually. While doing so we will develop abbreviations called *notations*, like the extension of the Einstein convention to integrals, and we will prove *necessary conditions* that must be satisfied by the wave invariants.

For example, we will show that the partial wave invariants do not depend on the connection but must contain the potential.

Lemma 4.37 (Necessary Condition 1).
The partial wave invariants $\mathsf{WI}_{k,l}(a, Q)$ are constant in $a \in \mathbb{R}^{n'}$.

Because the partial wave invariants do not depend on a we can write

$$\mathsf{WI}_{k,l}(Q) := \mathsf{WI}_{k,l}(0, Q)\,.$$

Lemma 4.40 (Necessary Condition 2).
Let $k \in \mathbb{N}$ and $l \in \mathcal{L}\backslash\{0\}$. Those summands in the partial wave invariant $\mathsf{WI}_{k,l}(Q)$ that do not contain the potential Q cancel, more precisely

$$\mathsf{WI}_{k,l}(0) = 0\,.$$

It will follow from these conditions that if all connections are isospectral with respect to a given potential Q then all partial wave invariants of this potential must vanish,

$$\mathsf{WI}_{k,l}(Q) = 0 \qquad \text{for all } k \in \mathbb{N} \text{ and all } l \in \mathcal{L},$$

see Corollary 4.39.

Both the notations and the necessary conditions are very important to the MATHEMATICA computation of the wave invariants. This MATHEMATICA notebook is central to this work and can be found in Appendix D and in digital form in [Ber18]. The results of those computations with the needed notation are given in Chapter 5. For example, by Theorem 5.6

$$\begin{aligned}\mathsf{WI}_{3,l}(Q) = Q_{-Fl}\Big(\mathrm{i}|l|^3\big(\frac{\tilde{F}_2}{96} - \frac{\tilde{F}_2(l,l)^2}{2304}\big) - \frac{n_{1,7}}{256|l|}\mathrm{i} + \frac{\mathrm{i}|l|n_{5,7}}{384}\tilde{F}_2(l,l)\Big) \\ + \sum_{c\in l[0,0]}^{Q}\Big(\frac{\mathrm{i}}{192}|l|^3\,\mathrm{Tr}\,\tilde{c}^2 + \frac{n_{5,7}\mathrm{i}}{64}|l|\Big) - \sum_{c\in l[c_1,-c_1]}^{Q}\frac{\mathrm{i}|l|^3\tilde{c}_{1,2}}{8\tilde{c}_1(l)^2} - \sum_{c\in l[0,0,0]}^{Q}\frac{\mathrm{i}|l|^3}{48}\,.\end{aligned}$$

The wave invariants can be combined to give somewhat shorter *small wave invariants* and of those the first five are shown in Theorem 5.8. Although the intermediate expressions contain thousands to millions of summands, the final expressions for the wave invariants are reasonably short and readable.

Following this chapter describing the wave invariants we will give applications of these invariants to our initial spectral problem in Chapter 6. We

show that for all lattices and nondegenerate line bundles we can always find a single potential that determines the class of connections isospectral to some given connection to any degree we choose.

Theorem 6.4. For any lattice $\mathcal{L}$ and any two natural numbers $N_1 \in \mathbb{N}$ and $0 \leq N_2 < n$ we can find a smooth real-valued potential $Q \in C^\infty(M)$ such that the set of isospectral translation-invariant connections in $\mathbb{R}^{n\prime}/\mathcal{L}'$ consists of exactly N_1 smooth deformations with N_2 degrees of freedom.

More precisely, with the basis $(X_1, \dots, X_n) \coloneqq (U_1, \dots, U_m, V_1, \dots, V_m)$ of $\mathbb{R}^n$ we can choose Q such that for all connections $a \in \mathbb{R}^{n\prime}$

$$\mathrm{Iso}(a) = \left\{ [a + \frac{i}{N_1} X^1 + \alpha_1 X^{n-N_2+1} + \cdots + \alpha_{N_2} X^n] \mid i \in \mathbb{Z},\ \alpha_1, \dots, \alpha_{N_2} \in \mathbb{R} \right\}$$

within $\mathbb{R}^{n\prime}/\mathcal{L}'$.

In particular, there exists a potential such that each translation-invariant connection a is spectrally determined.

We will also prove the converse to the transplantations above: For certain potentials two connections $a, b \in \mathbb{R}^{n\prime}$ can be isospectral only if (Q, a, b) is of type (P) or of type (M). One of those results, namely Lemma 6.12, requires and uses the fifth wave invariant where the first four wave invariants do not give any information. We give concrete examples for those results.

We also ask more generally: Do there always exist nonisospectral connections at all? All connections are isospectral if Q is constant. Also, if they are all isospectral then all partial wave invariants must vanish.

Conjecture 6.18. For any flat torus $M = \mathbb{R}^n/\mathcal{L}$ with a line bundle given by some Chern invariant factors $r_1 \mid \cdots \mid r_{n/2}$ and for any smooth real-valued *nonconstant* potential $Q \in C^\infty(M)$ there exist nonisospectral translation-invariant connections.

If all Chern invariant factors are one, this conjecture is rather trivial. On the other hand, we can find for any $K \in \mathbb{N}$ a combination of nonconstant potential and Chern invariant factors such that the first K wave invariants are zero, see Theorem 6.20. In other words, the information provided by finitely many wave invariants is limited and we cannot expect to prove the conjecture from the first five wave invariants.

However, if the potential has *extremal frequencies*, for example if the lattice support $\left\{ c \in \mathcal{L}' \mid Q_c = \langle Q, E_c \rangle_{\mathrm{L}^2(M)} \neq 0 \right\}$ is finite, then the conjecture holds.

Theorem 6.24. For every nonconstant potential $Q \in C^\infty(M)$ with an extremal frequency there exists a lattice vector $l \in \mathcal{L}\backslash\{0\}$ such that the partial wave invariant $\mathsf{WI}_{r_m,l}(Q)$ is nonzero. In particular, there exist nonisospectral translation-invariant connections.

This Theorem will follow from general properties, the necessary conditions, of the wave invariant and not from the first five wave invariants.

Finally, [GGKW08] contains a sign error that causes their wave invariant to be not spectrally invariant. We show in Section 6.5 that the results, which they prove using the wave invariants, are true regardless; we even show a slight generalization. The reason why the sign error has no effect on the results are given in Remarks 4.33 and 4.49.

Let us point out that the most difficult part of this thesis is the computation of certain τ-integrals appearing in the wave invariants. While it is not difficult to integrate particular τ-integrals manually we do need the general algorithm to integrate all appearing integrals given in Appendix B. This algorithm is based on the relatively elementary Lemma B.7. The case distinction in this Lemma causes the quite complicated combinatorics resulting in the *Q-sums* over *cases*.

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Chapter 1

Setting and Notation

In this Thesis we will study Schrödinger operators acting on sections of nondegenerate Hermitian line bundles over flat tori. In this chapter these line bundles will be introduced.

We will give a normal form for the nondegenerate line bundles that will be particularly suitable for calculations and that will enable us to explicitly compute wave invariants.

In my diploma thesis [Ber17] I have studied the isospectrality of these Schrödinger operators with a particular focus on transplantations of potentials. This introduction is a condensed version of the first half of this thesis and more explanations description of the following concepts can be found there.

1.1 Flat Tori and Line Bundles

Flat tori are the quotient of $\mathbb{R}^n$ by a lattice equipped with a the canonical, flat metric. The line bundles over those tori will be assumed to have nondegenerate Chern classes. This demand will require the dimensions of the tori to be even.

Definition 1.1 (Lattice).
If $(X_1, \dots, X_n)$ is a basis of $\mathbb{R}^n$, then $\mathcal{L} := \mathbb{Z}(X_1, \dots, X_n)$ is called a *lattice*. The *unit cell* of the lattice $\mathcal{L}$ with respect to a given basis is the compact set $\{\sum_i \alpha_i X_i \mid \alpha_i \in [0,1]\}$.

Definition 1.2 (Flat torus).
A lattice $\mathcal{L}$ forms a group and acts on $\mathbb{R}^n$ via the addition $+$. Every *translation* by some $l \in \mathcal{L}$

$$T_l \colon \mathbb{R}^n \ni x \mapsto l + x \in \mathbb{R}^n$$

is an isometry and thus $\mathcal{L}$ is a group of isometries acting on $\mathbb{R}^n$. Let

$$\pi_{\mathcal{L}} \colon \mathbb{R}^n \to \mathcal{L}\backslash\mathbb{R}^n =: M$$

be the projection to the quotient space endowed with the quotient topology. There is exactly one Riemannian metric $\langle .\,, . \rangle_{\mathcal{L}}$ on M such that $\pi_{\mathcal{L}}$ is a Riemannian covering, where $\mathbb{R}^n$ is equipped with the standard metric $\langle .\,, . \rangle$. The Riemannian manifold $(M, \langle .\,, . \rangle_{\mathcal{L}})$ is called *flat torus*.

Definition 1.3. Every translation T_x on $\mathbb{R}^n$ by an $x \in \mathbb{R}^n$ descends to an isometry on the torus. A differential form on $M = \mathcal{L}\backslash\mathbb{R}^n$ is called *translation-invariant* if it lifts to a form which is invariant under the group of those isometries.

Flat tori are closed and orientable and thus the Laplace-Beltrami operator $\Delta_{\mathrm{LB}} \coloneqq \delta \mathrm{d} + \mathrm{d}\delta$ on functions and forms exists. A function or differential form ω is called harmonic if $\Delta_{\mathrm{LB}}\omega = 0$.

Lemma 1.4. A differentiable form on a flat torus is translation-invariant if and only if it is harmonic.

Proof. Obviously, every translation-invariant form is also harmonic. Since M is closed, Green's formula reads

$$\int_M \langle \operatorname{grad} h, \operatorname{grad} f \rangle - h \cdot \Delta_{\mathrm{LB}} f \, \mathrm{d}V = 0 \qquad \text{for all } h, f \in C^\infty(M).$$

For a harmonic function f and $h \coloneqq f$ we obtain $\int_M \|\operatorname{grad} f\|^2 \, \mathrm{d}V = 0$ and thus $\operatorname{grad} f = 0$. Hence, f is translation-invariant.

Now, let $\omega = \sum_{i_1<\cdots<i_p} \omega_{i_1,\ldots,i_p} \mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_p}$ be a p-form in the standard local coordinates. With

$$\Delta_{\mathrm{LB}}\omega = \sum_{i_1<\cdots<i_p} (\Delta_{\mathrm{LB}}\omega_{i_1,\ldots,i_p}) \, \mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_p} \,.$$

we have that if ω is harmonic, then so are its components. This means that the components and therefore ω itself are translation-invariant. □

Remark 1.5. Let $\{e_i\}$ denote the standard basis of $\mathbb{R}^n$ and $(x^1, \ldots, x^n)$ the corresponding coordinates. If $U \subset \mathbb{R}^n$ is the interior of a unit cell, then the standard coordinates descend to coordinates on $\pi_{\mathcal{L}}(U)$ and thus we obtain a basis $\{\frac{\partial}{\partial x^i}\}$ on every $\mathrm{T}_x M$ with $x \in U$.

A translation-invariant p-form A on M is defined already by any single $A_x \colon (\mathrm{T}_x M)^p \to \mathbb{R}$. When identifying the tangent space $\mathrm{T}_x M$ with $\mathbb{R}^n$ via the map $\frac{\partial}{\partial x^i} \mapsto e_i$, we can identify the translation-invariant p-form A with an element of $\Lambda^p(\mathbb{R}^n)$, that is, an antisymmetric p-linear map on $\mathbb{R}^n$.

This identification will be of great importance later in this work because we will study connections which are determined by harmonic forms. Before that, the following observation about the harmonic representative of a Chern class will be very useful.

The following 2-form F was called Ω in [Ber17]. Latin letters are, however, more convenient to use in MATHEMATICA notebooks.

Remark 1.6. The vector bundle isomorphism classes of complex line bundles λ over M are classified by their Chern classes $c(\lambda) \in \check{\mathrm{H}}^2(M, \mathbb{Z})$. By the Čech-de Rham isomorphism $\check{\mathrm{H}}^p(M, \mathbb{R}) \cong \mathrm{H}^p_{\mathrm{dR}}(M)$, the class $c(\lambda)$ can be interpreted as an element of $\mathrm{H}^2_{\mathrm{dR}}(M)$. For such a de Rham cohomology class there exists a unique harmonic differential form F on M with $c(\lambda) = [F]$.

If F is this harmonic representative of $c(\lambda)$, then F can be considered as an antisymmetric bilinear map $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ with $F(\mathcal{L} \times \mathcal{L}) \subset \mathbb{Z}$.

Proof. Two linearly independent lattice vectors $l, k \in \mathcal{L}$ span a parallelepiped in $\mathbb{R}^n$. Its projection $P \subset M$ is a closed 2-chain in the singular homology of M. The class $[F]$ can be seen as an element of the corresponding cohomology and we can show that the de Rham isomorphism is given by integration. Thus:

$$F(l, k) = \int_P [F] = [F](P) \in \mathbb{Z}$$

Confer [Lee02, Chapter 16] or [War83, Chapter 5]. □

The following lemma is well-known, we include a proof for the convenience of the reader.

Lemma 1.7. If $F\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a nondegenerate antisymmetric bilinear map with $F(\mathcal{L} \times \mathcal{L}) \subset \mathbb{Z}$, then $n = 2m$ is an even integer and there exists one and only one tuple $(r_1, \dots, r_m) \in \mathbb{N}^m$ such that

(a) there exists a lattice basis $\mathfrak{B} \coloneqq \{U_1, \dots, U_m, V_1, \dots, V_m\}$ of $\mathcal{L}$ with $F(U_i, V_j) = r_i \cdot \delta_{ij}$ and $F(U_i, U_j) = F(V_i, V_j) = 0$ for $i, j = 1, \dots, m$ and

(b) $r_1 \mid r_2 \mid \cdots \mid r_m$.

If $\{u^1, \dots, u^m, v^1, \dots, v^m\}$ are the coordinates corresponding to the basis $\mathfrak{B}$, then $F = \sum_i r_i \, \mathrm{d}u^i \wedge \mathrm{d}v^i$. The integers r_i are called *Chern invariant factors* and every such basis $\mathfrak{B}$ shall be called *Chern basis*.

Proof. For every $U \in \mathcal{L}$ the set $\mathfrak{a}_U \coloneqq \{F(U, V) \mid V \in \mathcal{L}\} \subset \mathbb{Z}$ is an ideal and, since $\mathbb{Z}$ is a principal ideal domain, $\mathfrak{a}_U = d_U\mathbb{Z}$ for some $d_U \in \mathbb{Z}$. Since F is nondegenerate, we can assume $d_U > 0$ for $U \neq 0$ and thus $r_1 \coloneqq \min\left\{d_U \mid U \in \mathcal{L}\backslash\{0\}\right\} > 0$. Choose U_1 and V_1 such that $F(U_1, V_1) = r_1$.

By construction r_1 divides both $F(U, U_1)$ and $F(U, V_1)$ for every $U \in \mathcal{L}$; in particular

$$U + \frac{F(U,U_1)}{r_1} V_1 - \frac{F(U,V_1)}{r_1} U_1 \in \mathcal{L}_{n-2}\,,$$

where $\mathcal{L}_{n-2}$ is the orthogonal complement with respect to F of $\mathbb{Z}(U_1, V_1)$ in $\mathcal{L}$. This means that $\mathcal{L} = \mathbb{Z}(U_1, V_1) \oplus \mathcal{L}_{n-2}$ and that $\mathcal{L}_{n-2}$ is a lattice of dimension $n-2$ in $\mathbb{Z}(U_1, V_1)^\perp = \mathbb{R} \cdot \mathcal{L}_{n-2}$, where $\perp$ is to be understood with respect to F.

The restriction of F to $\mathbb{R} \cdot \mathcal{L}_{n-2}$ is again nondegenerate, and repeating this process with $\mathcal{L}_{n-2}$ inductively gives a tuple $(r_1, \dots, r_m)$ of integers with the corresponding lattice basis $(U_1, \dots, U_m, V_1, \dots, V_m)$. In particular, $n = 2m$ is even.

Now assume (without loss of generality) that $r_1 \nmid r_2$, i. e. there is an $a \in \mathbb{Z}$ such that $0 < r_2 - a r_1 < r_1$. This implies

$$\begin{aligned} 0 < F(U_2, V_2) - aF(U_1, V_1) = \\ F(U_2, V_1 + V_2) - aF(U_1, V_1 + V_2) = F(U_2 - aU_1, V_1 + V_2) < r_1\,, \end{aligned}$$

which contradicts the choice of r_1.

It remains to show that the tuple r is unique. Let $F^i := F \wedge \cdots \wedge F$. This is an alternating $2i$-linear form and, if we choose pairwise distinct indices $k_1, \dots, k_i \in \{1, \dots, m\}$, then

$$F^i(U_{k_1}, V_{k_1}, \dots, U_{k_i}, V_{k_i}) = i! \cdot r_{k_1} \cdots r_{k_i}\,.$$

When applied to any other combination of $2i$ vectors in $\{U_i, V_i\}$ the form vanishes. Therefore, for every $2i$-tuple $(X_1, \dots, X_{2i}) \in \mathcal{L}^{2i}$ there are integers $\beta_{k_1 \cdots k_i}$ with

$$F^i(X_1, \dots, X_{2i}) = \sum_{k_1 < \cdots < k_i} \beta_{k_1 \cdots k_i} \cdot i! \cdot r_{k_1} \cdots r_{k_i}\,.$$

Since $r_1 \mid \cdots \mid r_m$, the product $i! \cdot r_1 \cdots r_i$ divides all summands and there is a suitable $N \in \mathbb{N}$ with $|F^i(W_1, \dots, W_{2i})| = i! \cdot r_1 \cdots r_i \cdot N$.

This means $i! \cdot r_1 \cdots r_i$ is the minimum of the nonzero values of $|F^i|$ on $\mathcal{L}^{2i}$. This characterizes the invariants r_i of F. □

Conclusion 1.8. The line bundles λ over M are classified, up to isomorphism, by their Chern classes $c(\lambda) \in \check{\mathrm{H}}^2(M, \mathbb{Z})$, and those classes can be identified with antisymmetric bilinear maps F on $\mathbb{R}^n \times \mathbb{R}^n$ taking integer values on the lattice. If F is nondegenerate, then the line bundle is said to have a *nondegenerate Chern class* or just to be *nondegenerate*. In this case we also obtain a normal form of F.

In the following this normal form is used to construct an explicit representative for every isomorphism class of nondegenerate line bundles over a given flat torus.

Definition 1.9. For any given class $[F] \in \check{\mathrm{H}}^2(M, \mathbb{Z})$ use its Chern invariant factors r_i and a fixed Chern basis $\mathfrak{B}$ to define for $x, y \in \mathbb{R}^n$:

$$w_x(y) \coloneqq \sum_{i=1}^{m} r_i u^i(x) v^i(y) \qquad \text{and} \qquad e_x(y) \coloneqq \mathrm{e}^{2\pi \mathrm{i} \cdot w_x(y)} \in \mathrm{U}(1)\,,$$

where $\{u^i, v^i\}$ are the coordinates corresponding to the Chern basis. Also define an action of the group $\mathcal{L}$ on the total space $\mathbb{R}^n \times \mathbb{C}$ of the trivial line bundle θ^1 over $\mathbb{R}^n$ via

$$l\,.\,(x,z) \coloneqq (l + x,\, e_l(x) \cdot z) \qquad \text{for } l \in \mathcal{L},\, x \in \mathbb{R}^n \text{ and } z \in \mathbb{C}.$$

Define a bundle $\omega \coloneqq (L_\omega, \pi_\omega, M)$ over M by setting $L_\omega \coloneqq \mathcal{L}\backslash(\mathbb{R}^n \times \mathbb{C})$ and $\pi_\omega \colon L_\omega \ni [x,z] \mapsto [x] \in \mathcal{L}\backslash\mathbb{R}^n = M$. ω is a Hermitian complex line bundle over M, where the Hermitian structure is induced by the standard Hermitian product of the trivial bundle. Moreover, ω pulls back to the trivial bundle over $\mathbb{R}^n$ under the canonical projection $\mathbb{R}^n \to \mathcal{L}\backslash\mathbb{R}^n$.

Remark 1.10. Denote the space of smooth sections of a line bundle λ by $\mathcal{E}(\lambda)$. A section $s \in \mathcal{E}(\theta)$ of the trivial line bundle θ^1 over $\mathbb{R}^n$ has the form $s(x) = (x, f(x))$ with a function $f \in C^\infty(\mathbb{R}^n, \mathbb{C})$. A similar statement holds for sections $\mathcal{E}(\omega)$ of ω, but the function must be $\mathcal{L}$-equivariant: A function $f \in C^\infty(\mathbb{R}^n, \mathbb{C})$ represents a section of ω if and only if it satisfies

$$f(x + l) = e_l(x) \cdot f(x) \qquad \text{for every } x \in \mathbb{R}^n \text{ and } l \in \mathcal{L}.$$

The space of sections of ω is isomorphic to

$$C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \coloneqq \{f \in C^\infty(\mathbb{R}^n, \mathbb{C}) \mid f(\,.\,+ l) = e_l \cdot f \quad \text{for all } l \in \mathcal{L}\}$$
$$\mathcal{E}(\omega) \cong \mathcal{E}(\theta)^{\mathcal{L}} \cong C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}}\,.$$

In the following we shall identify sections with the corresponding functions. For example, it is understood that for a vector field X and a section $s(x) = (x, f(x))$

$$X_x(s) = (x, X_x(f))\,.$$

Similarly, a vector field $X \in \mathcal{X}(\mathbb{R}^n)$ descends to a vector field on M if and only if it is $\mathcal{L}$-equivariant: $T_{l*}X = X_{T_l}$.

Definition 1.11. For every complex-valued 1-form A on $\mathbb{R}^n$ we obtain a *connection* on the trivial bundle θ^1 over $\mathbb{R}^n$ by setting

$$\nabla := \mathrm{d} + A\,, \qquad \text{which means that for any vector field } X \in \mathcal{X}(\mathbb{R}^n)$$
$$\big(\nabla_X s\big)(x) = \big(x, X_x(f) + A_x(X)\cdot f(x)\big)$$

for every section $s(x) = (x, f(x))$ of the trivial line bundle. Also, every connection on θ^1 has this form. A connection ∇ on θ^1 descends to a connection on ω, also called ∇, if and only if it maps $\mathcal{L}$-equivariant sections to $\mathcal{L}$-equivariant sections. More precisely, for every $\mathcal{L}$-equivariant section s of the trivial bundle and every $\mathcal{L}$-equivariant $X \in \mathcal{X}(\mathbb{R}^n)$ the connection must satisfy

$$\big(\nabla_X s\big)(l + x) = l\,.\big(\nabla_X s\big)(x) \qquad \text{for all } x \in \mathbb{R}^n \text{ and } l \in \mathcal{L}.$$

Lemma 1.12. ∇ descends to a connection on ω if and only if

$$T_l^* A = A - 2\pi\mathrm{i} w_l \qquad \text{for all } l \in \mathcal{L}.$$

Proof. Note that using the canonical isomorphism identifying $\mathbb{R}^n$ with all its tangent spaces we can consider w_l as a function and as a 1-form on $\mathbb{R}^n$ and for $X \in \mathcal{X}(\mathbb{R}^n)$ we have $X(w_l) = w_l(X)$. Assuming A satisfies the given equation we have for any $\mathcal{L}$-equivariant section s (of ω) and $X \in \mathcal{X}(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$:

$$A_{T_l(x)}(X)\cdot s(x+l) = (T_l^* A)_x(X)\cdot e_l(x)\cdot s(x) = \\ e_l(x)\cdot\big(A_x(X)\cdot s(x) - s(x)\cdot 2\pi\mathrm{i} w_l(X_x)\big)$$

and with

$$X_{x+l}(s) = X_x(s\circ T_l) = X_x(e_l\cdot s) = e_l(x)\cdot\big(X_x(s) + s(x)\cdot 2\pi\mathrm{i} w_l(X_x)\big)$$

it follows that $\nabla_X s$ is $\mathcal{L}$-equivariant:

$$(\nabla_X s)\circ T_l = X_{T_l}(s) + A_{T_l}(X)\cdot(s\circ T_l) = e_l\cdot\big(X(s) + A(X)\cdot s\big) = l\,.\nabla_X s\,.$$

Reasoning backwards gives the converse. □

Further, a connection is compatible with the Hermitian product on the trivial bundle,

$$X.\langle s, t\rangle = \langle \nabla_X s, t\rangle + \langle s, \nabla_X t\rangle\,,$$

if and only if the 1-form A is purely imaginary, i. e. $A_x(X) \in \mathrm{i}\mathbb{R}$ for all $x \in \mathbb{R}^n$ and all $X \in \mathrm{T}_x\mathbb{R}^n$.

Definition 1.13. For convenience let us define a *distinguished connection* ∇^{D} on ω through

$$A^{\mathrm{D}}_x := -2\pi\mathrm{i}\, w_x \qquad \text{for all } x \in \mathbb{R}^n.$$

This connection is Hermitian.

To avoid the proliferation of factors $2\pi\mathrm{i}$ we introduce the following notation.

Definition 1.14. For any a set

$$\tilde{a} := 2\pi\mathrm{i} \cdot a\,.$$

With this notation we have the following relation between A^{D} and F.

Lemma 1.15. $\quad A^{\mathrm{D}}_X(Y) - A^{\mathrm{D}}_Y(X) = -\tilde{F}(X,Y)$

Proof. Both sides are bilinear and it is sufficient to show the claim for $X = U_1$ and $Y = V_1$. Then,

$$A^{\mathrm{D}}_{U_1}(V_1) - A^{\mathrm{D}}_{V_1}(U_1) = -2\pi\mathrm{i}r_1 = -2\pi\mathrm{i}F(U_1,V_1) = -\tilde{F}(U_1,V_1)\,. \qquad \square$$

This connection is very useful as every connection on ω is equal to this connection plus some 1-form on the torus. But before studying this, the distinguished connection will be used to calculate the harmonic representative of the Chern class of ω.

Lemma 1.16. The Chern class $c(\omega)$ is represented by F.

Proof. Under the Čech-de Rham isomorphism the Chern class is represented by $-\frac{1}{2\pi\mathrm{i}}\kappa$, where κ is the curvature form of any connection on ω. Let e be a local frame of the trivial bundle θ^1 over $\mathbb{R}^n$ such that $\mathrm{d}(e) = 0$. The connection form of the distinguished connection with respect to this frame is A^{D} and the Cartan structure equation yields

$$\kappa = \mathrm{d}A^{\mathrm{D}} = -2\pi\mathrm{i}\sum_{i=1}^{m} r_i\, \mathrm{d}u^i \wedge \mathrm{d}v^i = -2\pi\mathrm{i}F\,.$$

$\square$

Overall this shows that every nondegenerate line bundle over the flat torus $M = \mathcal{L}\backslash\mathbb{R}^n$ is isomorphic to an ω as constructed above.

1.2 Connections

The Laplacians and their spectra considered later will be constructed from connections on ω. Thus, it is important to know these connections. Their number can be reduced by excluding some of them from our considerations and by introducing an equivalence relation on the remaining ones. The classes of this equivalence relation will have very simple representatives.

Remark 1.17. Every connection ∇ on the line bundle ω has the form

$$\nabla = \nabla^{\mathrm{D}} + B \qquad \text{with} \qquad B = a + \mathrm{d}b + \mathrm{d}^* c\,,$$

where ∇^{D} is the distinguished connection and B is a 1-form on M split up by Hodge decomposition into a direct sum of a harmonic 1-form a, an exact part given by a function $b \in C^\infty(M, \mathbb{C})$ and a coexact part given by a 2-form c. If the connection is Hermitian, then B as well as a, b and c are imaginary-valued.

In particular, the form B can be pulled back to a form in $\Omega^1(\mathbb{R}^n, \mathbb{C})$ with $T_l^* B = B$. Conversely, for every translation-invariant such form B, $A^{\mathrm{D}} + B$ is a form with $T_l^*(A^{\mathrm{D}} + B) = A^{\mathrm{D}} + B - 2\pi i w_l$ and this means that the connection $\mathrm{d} + A^{\mathrm{D}} + B$ on θ^1 descends to a connection on ω, namely ∇. Therefore, there is a bijection between the connections on ω and the $\mathcal{L}$-invariant complex-valued 1-forms on $\mathbb{R}^n$.

Definition 1.18. A connection ∇ on a line bundle λ over M is called *translation-invariant* if its curvature form is invariant under translations.

This is not a meaningless definition; there are translation-invariant connections on every nondegenerate line bundle over any even-dimensional torus: At the end of the previous section it was shown that the curvature form of the distinguished connection is $-2\pi i F$, which is by definition harmonic and hence translation-invariant.

Proposition 1.19. All translation-invariant connections have the same curvature form. A connection $\nabla = \nabla^{\mathrm{D}} + B$ on ω is translation-invariant if and only if the coexact part of B vanishes, $\mathrm{d}^* c = 0$.

Proof. By the Cartan structure equation both curvature forms differ by $\mathrm{d}B = \mathrm{d}\mathrm{d}^* c$. If the coexact part of B vanishes, both curvature forms are equal and ∇ is translation-invariant, because ∇^{D} is. Conversely, if both connections are translation-invariant, $\mathrm{d}\mathrm{d}^* c$ must be harmonic. By Hodge decomposition $\mathrm{d}\mathrm{d}^* c = 0$. From this and $\mathrm{d}^*\mathrm{d}^* c = 0$ it follows that $\mathrm{d}^* c$ is harmonic. Again, by the Hodge decomposition $\mathrm{d}^* c = 0$. □

Definition 1.20. A *bundle automorphism* A of a line bundle λ is a bundle map such that: If s is a smooth section, then $A \circ s$ a smooth section and A is a linear automorphism on each fibre of λ. If λ is an Hermitian line bundle, then a bundle automorphism A of λ is called *Hermitian* if F is an isometric automorphism on each fibre.

Definition 1.21. Two connections ∇^1 and ∇^2 on a Hermitian line bundle λ over a manifold M are *gauge equivalent* if there is a Hermitian bundle automorphism A which *intertwines* the two connections:

$$\nabla^1_X \circ A = A \circ \nabla^2_X \qquad \text{for all } X \in \mathcal{X}(M).$$

Gauge equivalent connections will have the same spectrum and it will therefore be sufficient to consider only one preferably simple representative of each gauge equivalence class.

Definition 1.22. The *dual lattice* $\mathcal{L}' \subset \mathbb{R}^{n\prime}$ of the lattice $\mathcal{L}$ is the set of all linear functionals on $\mathbb{R}^n$ with integer values on $\mathcal{L}$. If $(X^1, \dots, X^n)$ is the dual basis of a basis $(X_1, \dots, X_n)$ of $\mathcal{L}$, i. e. $X^i(X_j) = \delta_{ij}$, then

$$\mathcal{L}' = \mathbb{Z}(X^1, \dots, X^n)$$

and therefore $\mathcal{L}'$ is indeed a lattice in $\mathbb{R}^{n\prime}$.

Proposition 1.23. The gauge equivalence class of a translation-invariant Hermitian connection $\nabla = \nabla^{\mathrm{D}} + B = \nabla^{\mathrm{D}} + \tilde{a} + \mathrm{d}b$ is independent of the function $b \in C^\infty(M, \mathrm{i}\mathbb{R})$ and depends solely on the class $[a] \in \mathbb{R}^{n\prime}/\mathcal{L}'$.

Proof. Given a connection $\nabla^b = \nabla^{\mathrm{D}} + \tilde{a} + \mathrm{d}b$ define a bundle map $A_b \colon \omega \to \omega$ through $L_\omega \ni [x, z] \mapsto [x, \mathrm{e}^{-b(x)}z] \in L_\omega$, which is a well-defined Hermitian bundle automorphism with inverse A_{-b}. Using this automorphism we can construct a new connection $\nabla \coloneqq A_b^{-1} \circ \nabla^b \circ A_b$ satisfying

$$\nabla s = A_b^{-1} \circ \nabla^b(\mathrm{e}^{-b}s) = A_b^{-1}(\mathrm{d}\mathrm{e}^{-b} \cdot s + \mathrm{e}^{-b}\nabla^b s) = -\mathrm{d}b \cdot s + \nabla^b s = (\nabla^{\mathrm{D}} + \tilde{a})s$$

for every $s \in \mathcal{E}(\omega)$. Thus, every translation-invariant connection ∇^b is gauge equivalent to a translation-invariant connection whose form has vanishing exact part.

As $\mathcal{L}'$ are the functionals on $\mathbb{R}^n$ with integer values on $\mathcal{L}$, we can argue similarly: For $a \in \mathcal{L}'$ there is a well-defined Hermitian bundle automorphism A_a via $L_\omega \ni [x, z] \mapsto [x, \mathrm{e}^{-\tilde{a}(x)}z] \in L_\omega$ and a new connection $A_a^{-1} \circ \nabla^b \circ A_a$, which differs from ∇^b by $\mathrm{d}\tilde{a} = \tilde{a}$. (The differential of the linear function $a \colon \mathbb{R}^n \to \mathbb{R}$ is equal to the harmonic 1-form a.) □

Notation 1.24. Since every translation-invariant connection is gauge equivalent to a connection of the form $\nabla^{\mathrm{D}} + \tilde{a}$ with $a \in \mathbb{R}^{n\prime}$ we will identify those connections with these 1-forms.

The following involutions were defined in [GGKW08, Definition 2.12], see also [GGKW08, Remark 2.19].

Definition 1.25. Define an involutive isometry $\check{}\colon \mathbb{R}^n \to \mathbb{R}^n$ by setting $\check{x} := -x$. This map descends to an involutive isometry $\check{}\colon M \to M$ of the torus M. Define a map on the smooth functions $C^\infty(\mathbb{R}^n, \mathbb{C})$ by setting $\check{f}(x) := f(\check{x})$. This map descends to a map on the functions on the torus M and to a map on the smooth sections $\mathcal{E}(\omega)$ of the line bundle ω. Further, denote the push-forward of $X \in \mathcal{X}(M)$ under the isometry $\check{}$ by $\check{X}$, which means $\check{X}_x(f) := X_{\check{x}}\check{f}$.

Using the involutions on vector fields and sections we can construct an involution on the set of connections on ω: For any connection ∇ on the line bundle ω we define a connection by

$$\check{\nabla}_X s := (\nabla_{\check{X}}\check{s})\check{} \qquad \text{for all } X \in \mathcal{X}(M) \text{ and every section } s.$$

Remark 1.26. The map $\mathcal{E}(\omega) \ni s \mapsto \check{s} \in \mathcal{E}(\omega)$ is indeed well-defined because $\check{s}$ is $\mathcal{L}$-equivariant: For all $x \in \mathbb{R}^n$ and $l \in \mathcal{L}$ we have

$$\check{s}\,(x + l) = s(-x - l) = s(-x) \cdot e_{-l}(-x) = \check{s}(x) \cdot e_l(x)\,.$$

Also, we have to show that $\check{\nabla}$ is indeed a connection. All involutions $\check{}$ are $\mathbb{C}$-linear and thus $\check{\nabla}$ is $\mathbb{C}$-bilinear. For all $f \in C^\infty(M, \mathbb{C})$ and $s \in \mathcal{E}(\omega)$ we have $(fs)\check{} = \check{f}\check{s}$ and $(\check{X}\check{f})\check{} = X(f)$. If f is real-valued and $X \in \mathcal{X}(M)$, then $(fX)\check{} = \check{f}\check{X}$ and hence

$$\begin{aligned}
&\check{\nabla}_X fs = (\nabla_{\check{X}}\check{f}\check{s})\check{} = (\check{X}\check{f})\check{}\,\check{s} + \check{\check{f}}(\nabla_{\check{X}}\check{s})\check{} = X(f)s + f \cdot \check{\nabla}_X s \qquad \text{and}\\
&\check{\nabla}_{fX} s = (\nabla_{\check{f}\check{X}}\check{s})\check{} = (\check{f}\nabla_{\check{X}}\check{s})\check{} = f \cdot \check{\nabla}_X s \qquad \text{for all real-valued } f.
\end{aligned}$$

Thus, $\check{\nabla}$ is indeed a connection.

Definition 1.27. A connection ∇ on the line bundle ω over M is called $\mathbb{Z}_2$-*invariant* if $\nabla = \check{\nabla}$. A connection is called *weakly* $\mathbb{Z}_2$-*invariant* if $\nabla \sim \check{\nabla}$ with respect to gauge equivalence.

Lemma 1.28. A translation-invariant connection $\nabla^{\mathrm{D}} + \tilde{a}$ with a harmonic 1-form a is $\mathbb{Z}_2$-invariant if and only if $a = 0$. A translation-invariant connection $\nabla^{\mathrm{D}} + \tilde{a}$ is weakly $\mathbb{Z}_2$-invariant if and only if $a(\mathcal{L}) \subset \frac{1}{2}\mathbb{Z}$.

Proof. By Remark 1.17 every connection on the line bundle ω has the form $\nabla^{\mathrm{D}} + \tilde{a} + \mathrm{d}b + \mathrm{d}^* c$, where a is a harmonic 1-form. For a translation-invariant connection $\mathrm{d}^* c$ vanishes by Propositions 1.19 and the gauge equivalence class of the connection is independent of b by Proposition 1.23.

Assume we are given a connection $\nabla = \mathrm{d} + A$ with some 1-form A on M and an arbitrary tangent vector $X_x \in \mathrm{T}_x M$ at some point $x \in M$. Any tangent vector can be extended to a translation-invariant vector field on M: $X_y \coloneqq T_{y-x*} X_x$, where T_{y-x} is one of the translations acting on M with $x \mapsto y$. With this vector field we have for any section s that $\nabla_X s(x) = X_x(s) + A_x(X)s(x)$ and

$$(\check{\nabla}_X s)(x) = (\nabla_{\check{X}} \check{s})(\check{x}) = \check{X}_{\check{x}}(\check{s}) + A_{\check{x}}(\check{X})\check{s}(\check{x}) = X_x(s) + A_{-x}(-X)s(x).$$

Therefore, the connection $\mathrm{d} + A$ is $\mathbb{Z}_2$-invariant if and only if $A_x(X) = A_{-x}(-X)$. By Definition 1.9 and Definition 1.13 we have $A^{\mathrm{D}}_x(X) = A^{\mathrm{D}}_{-x}(-X)$, which implies that the distinguished connection is $\mathbb{Z}_2$-invariant. Thus, a connection $\nabla^{\mathrm{D}} + \tilde{a}$ for some harmonic 1-form a is $\mathbb{Z}_2$-invariant if and only if $a_x(X) = a_{-x}(-X) = a_x(-X)$, because every harmonic 1-form on a torus M is translation-invariant. Hence, $\nabla^{\mathrm{D}} + \tilde{a}$ is $\mathbb{Z}_2$-invariant if and only if $a = 0$.

To prove the second claim note first that $(\nabla^{\mathrm{D}} + \tilde{a})\check{}_X s = \nabla^{\mathrm{D}}_X s + \tilde{a}(\check{X})s$. This implies with $a(\check{X}) = -a(X)$ that a connection $\nabla^{\mathrm{D}} + \tilde{a}$ is weakly $\mathbb{Z}_2$-invariant if and only if there is an Hermitian bundle automorphism $\Phi\colon \omega \to \omega$ with

$$\Phi^{-1} \circ (\nabla^{\mathrm{D}} + \tilde{a}) \circ \Phi = \nabla^{\mathrm{D}} - \tilde{a}\,.$$

Every Hermitian bundle automorphism on ω has the form

$$\Phi[x, z] = [x, \mathrm{e}^{2\pi\mathrm{i}(\alpha(x) + h(x))} \cdot z]$$

for all elements $[x, z]$ in the total space L_ω of ω, see Definition 1.9. Here $\alpha \in \mathcal{L}'$ and h is an $\mathcal{L}$-periodic function on $\mathbb{R}^n$ and

$$\Phi^{-1} \circ (\nabla^{\mathrm{D}} + \tilde{a}) \circ \Phi s = \Phi^{-1}\Big(\mathrm{d}(\mathrm{e}^{2\pi\mathrm{i}(\alpha+h)} s) + (A^{\mathrm{D}} + \tilde{a})\mathrm{e}^{2\pi\mathrm{i}(\alpha+h)} s\Big) = \Big(\mathrm{d}s + 2\pi\mathrm{i}(\mathrm{d}\alpha + \mathrm{d}h)s + (A^{\mathrm{D}} + \tilde{a})s\Big).$$

Since the exterior differential of the linear function $\alpha \in C^\infty(\mathbb{R}^n)$ is equal to the harmonic 1-form α, $\mathrm{d}\alpha = \alpha$, the automorphism Φ intertwines the connection $\nabla^{\mathrm{D}} + \tilde{a}$ with the connection $\nabla^{\mathrm{D}} + \tilde{a} + 2\pi\mathrm{i}(\alpha + \mathrm{d}h)$. It follows that $\nabla^{\mathrm{D}} + \tilde{a}$ is weakly $\mathbb{Z}_2$-invariant if and only if there are an $\alpha \in \mathcal{L}'$ and an $\mathcal{L}$-periodic function $h \in C^\infty(\mathbb{R}^n)$ with $a + \alpha + \mathrm{d}h = -a$. By Hodge decomposition $\mathrm{d}h$ must vanish and therefore $\nabla^{\mathrm{D}} + \tilde{a}$ is weakly $\mathbb{Z}_2$-invariant if and only if there exists an $\alpha \in \mathcal{L}'$ with $2a = -\alpha$. □

Remark 1.29. Note that the distinguished connection ∇^{D} is the unique (up to gauge equivalence) translation- and $\mathbb{Z}_2$-invariant connection on ω. However, there are 2^n different gauge equivalence classes of translation- and weakly $\mathbb{Z}_2$-invariant connections.

1.3 The Laplacian and Spectra

In this section we will construct the Laplacian of a connection, introduce potentials and define their spectra.

Remark 1.30. Let ∇^{LC} denote the Levi-Civita connection over the flat torus $(M, \langle .\,, . \rangle_{\mathcal{L}})$. Generally, a connection on a vector bundle ξ over M may be seen as a map

$$\nabla^{\xi} \colon \mathcal{E}(\xi) \to \mathcal{E}(\mathrm{T}^*M \otimes \xi)\,.$$

With the help of the Levi-Civita connection we can construct a connection ∇^{T^*M} on the cotangent bundle T^*M via

$$\left(\nabla^{\mathrm{T}^*M}_X \mu\right)(Y) \coloneqq X.\mu(Y) - \mu(\nabla^{\mathrm{LC}}_X Y)$$

and a connection $\nabla^{\mathrm{T}^*M\otimes\xi}$ on the product bundle $\mathrm{T}^*M \otimes \xi$ by setting

$$\nabla^{\mathrm{T}^*M\otimes\xi}_X(\mu \otimes \eta) \coloneqq (\nabla^{\mathrm{T}^*M}_X \mu) \otimes \eta + \mu \otimes (\nabla^{\xi}_X \eta)\,.$$

With those connections we have a "second derivative"

$$\nabla^2 = \nabla^{\mathrm{T}^*M\otimes\xi} \circ \nabla^{\xi} \colon \mathcal{E}(\xi) \to \mathcal{E}(\mathrm{T}^*M \otimes \mathrm{T}^*M \otimes \xi)\,, \qquad \text{which satisfies}$$
$$\left(\nabla^{\mathrm{T}^*M\otimes\xi} \circ \nabla^{\xi} s\right)(X, Y) = \nabla^{\xi}_X \circ \nabla^{\xi}_Y s - \nabla^{\xi}_{\nabla^{\mathrm{LC}}_X Y} s$$

for all $X, Y \in \mathcal{X}(M)$ and every section $s \in \mathcal{E}(\xi)$.

Proof. If $\{X_i\}$ is a local frame of $\mathrm{T}M$ and $\{\omega_i\}$ its dual frame, then $\nabla^{\xi} s = \sum_i \omega_i \otimes \nabla^{\xi}_{X_i} s$. The product rule for the covariant derivative on tensor products yields

$$\nabla^{\mathrm{T}^*M\otimes\xi} \circ \nabla^{\xi} s = \sum_{i=1}^{n} \left(\left(\nabla^{\mathrm{T}^*M} \omega_i\right) \otimes \nabla^{\xi}_{X_i} s + \omega_i \otimes \nabla^{\xi}\left(\nabla^{\xi}_{X_i} s\right) \right) \qquad \text{and thus}$$

$$\begin{aligned}\left(\nabla^{\mathrm{T}^*M\otimes\xi} \circ \nabla^{\xi} s\right)(X_k, X_l) &= \sum_{i=1}^{n} -\omega_i\left(\nabla^{\mathrm{LC}}_{X_k} X_l\right) \nabla^{\xi}_{X_i} s + \nabla^{\xi}_{X_k} \circ \nabla^{\xi}_{X_l} s \\ &= \nabla^{\xi}_{X_k} \circ \nabla^{\xi}_{X_l} s - \sum_{i=1}^{n} \left(\omega_i \otimes \nabla^{\xi}_{X_i} s\right)\left(\nabla^{\mathrm{LC}}_{X_k} X_l\right) = \nabla^{\xi}_{X_k} \circ \nabla^{\xi}_{X_l} s - \nabla^{\xi}_{\nabla^{\mathrm{LC}}_{X_k} X_l} s\end{aligned}$$

Both sides of this equation are $C^\infty(M)$-linear in X_k and in X_l. Hence, this equation holds not only on the local frame $\{X_i\}$ but for all $X, Y \in \mathcal{X}(M)$. □

Remark 1.31. Given a connection ∇ on the line bundle ξ let

$$D^2_X \coloneqq \left(\nabla^2(X_i, X_j)\right)_{i,j=1\cdots n}$$

be the matrix of ∇^2 with respect to the local frame $X = \{X_i\}$. The entries of this matrix are the maps

$$\nabla^\xi_{X_k} \circ \nabla^\xi_{X_l} - \nabla^\xi_{\nabla^{\mathrm{LC}}_{X_k} X_l} \colon \mathcal{E}(\xi) \to \mathcal{E}(\xi)\,.$$

If $Y = \{Y_i\}$ is another local frame with transition matrix A, i. e. A is a matrix-valued function on M with $X_x = A_x Y_x$ for all $x \in M$, then the $C^\infty(M)$-bilinearity of the map $(X, Y) \mapsto \nabla^2(X, Y)$ yields $D^2_X = A D^2_Y A^T$. In particular, $\operatorname{trace} D^2_X = \operatorname{trace} D^2_Y A^T A$ and thus there is a well-defined trace of ∇^2 for all $\mathrm{O}(n)$-classes of frames.

Definition 1.32. Every connection ∇^λ on a line bundle λ over a flat torus M yields a *Laplacian* Δ acting on the sections of the line bundle λ. The Laplacian

$$\Delta \colon \mathcal{E}(\lambda) \to \mathcal{E}(\lambda) \qquad \text{is defined by} \qquad \Delta \coloneqq -\operatorname{trace} \nabla^2$$

with respect to the class of orthonormal frames. If X is such an orthonormal frame, then the Laplacian satisfies

$$\Delta = -\sum_{i=1}^{n} \left(\nabla^\lambda_{X_i} \circ \nabla^\lambda_{X_i} - \nabla^\lambda_{\nabla^{\mathrm{LC}}_{X_i} X_i} \right).$$

If we additionally assume that the frame field is translation-invariant, then $\nabla^{\mathrm{LC}}_{X_i} X_i = 0$, since $(M, \langle .\,, . \rangle_{\mathcal{L}})$ is flat, and thus

$$\Delta = -\sum_{i=1}^{n} \nabla^\lambda_{X_i} \circ \nabla^\lambda_{X_i}\,.$$

Definition 1.33. Every Hermitian connection ∇ on the line bundle ω constructed in Definition 1.9 can be pulled back to a connection $\mathrm{d} + A$ on the trivial bundle θ^1 with an imaginary-valued 1-form A. The corresponding Laplacian on ω shall be denoted by Δ_A. If $A = A^{\mathrm{D}} + \tilde{a}$, where A^{D} is the form of the distinguished connection and a a harmonic 1-form (see Definition 1.13 and Remark 1.17), we abbreviate $\Delta^{\mathrm{D}}_a \coloneqq \Delta_{A^{\mathrm{D}} + \tilde{a}}$.

Remark 1.34. The notions of Laplacians on ω and θ^1 are compatible in the following sense: If we pull back a connection ∇ on ω to the trivial bundle θ^1, then we obtain a Laplacian acting on $\mathcal{E}(\theta^1)$ by setting $\Delta^{\theta^1} \coloneqq -\operatorname{trace} \nabla^2 = -\sum_{i=1}^{n} \nabla_{X_i} \circ \nabla_{X_i}$, where $\{X_i\}$ is a translation-invariant orthonormal frame field. Since the connection comes from ω and the X_i are translation-invariant, ∇ commutes with the action of $\mathcal{L}$ on the sections $\mathcal{E}(\theta^1)$. Thus, Δ^{θ^1} commutes with that action and descends to a Laplacian on ω, namely Δ.

The following proposition illustrates how the Laplacians of connections differ from the usual Laplacian acting on functions. We use the identification of sections with $\mathcal{L}$-equivariant functions, see Remark 1.10.

Proposition 1.35. For every Hermitian connection $\nabla = \mathrm{d} + A$ on the line bundle ω over the flat torus $(M, \langle .\,, . \rangle_{\mathcal{L}})$ we have on $C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}}$

$$\Delta_A = -\Big(\operatorname{div} \circ \operatorname{grad} + \operatorname{div}(A^\#) + 2A \circ \operatorname{grad} - \|A\|^2\Big),$$

where the index-raising musical isomorphism $\#\colon \mathrm{T}^*M \to \mathrm{T}M$ is the inverse of the duality isomorphism $\flat\colon \mathrm{T}M \ni X \mapsto \langle X, . \rangle \in \mathrm{T}^*M$.

Proof. By definition we have for every $s \in \mathcal{E}(\omega) \cong C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}}$ and $X \in \mathcal{X}(M)$

$$\begin{aligned} -\nabla_X \circ \nabla_X s = -\nabla_X\Big(X(s) + A(X)s\Big) = \\ -\Big(X\Big(\mathrm{d}s(X)\Big) + X\Big(A(X)\Big)s + 2A(X)X(s) + A(X)^2 s\Big), \end{aligned}$$

where both A and X are pulled back to $\mathbb{R}^n$. By evaluating the four summands we obtain the desired formula:

Note that the gradient is defined via $\langle \operatorname{grad} s, X\rangle_{\mathcal{L}} = X(s)$, which means $\operatorname{grad} s = (\mathrm{d}s)^\#$. Thus, for the first two terms it suffices to show that $\operatorname{div} Y = \sum_i X_i\Big(Y^\flat(X_i)\Big)$ for any vector field Y and any translation-invariant orthonormal frame $\{X_i\}$.

The divergence is defined by $(\operatorname{div} Y)\,\mathrm{d}V = \mathrm{d}(Y \lrcorner\, \mathrm{d}V)$ and $\mathrm{d}V = X_1^\flat \wedge \cdots \wedge X_n^\flat$. With $Y = \sum_i Y^i X_i$

$$Y \lrcorner\, \mathrm{d}V = \sum_{i=1}^n Y^i (-1)^{i-1} X_1^\flat \wedge \cdots \wedge \widehat{X_i^\flat} \wedge \cdots \wedge X_n^\flat\,.$$

Since the $\{X_i\}$ are translation-invariant, $[X_i, X_j] = 0$ and hence

$$\begin{aligned} &\operatorname{div} Y = \mathrm{d}(Y \lrcorner\, \mathrm{d}V)(X_1, \ldots, X_n) \\ &= \sum_{i,l=1}^n (-1)^{i+l} X_l\Big(Y^i X_1^\flat \wedge \cdots \wedge \widehat{X_i^\flat} \wedge \cdots \wedge X_n^\flat\,(X_1, \ldots, \widehat{X_l}, \ldots, X_n)\Big) \\ &\qquad\qquad = \sum_{i=1}^n X_i\Big(Y^\flat(X_i)\Big) \end{aligned}$$

as $Y^\flat(X_i) = \langle Y, X_i\rangle = Y^i$. The third summand is given by

$$2\sum\nolimits_i A(X_i)X_i(s) = 2A\Big(\sum\nolimits_i \langle \operatorname{grad} s, X_i\rangle_{\mathcal{L}} X_i\Big) = 2A \circ \operatorname{grad} s\,.$$

Since A is imaginary-valued and satisfies $A = \sum_i A(X_i) X_i^\flat$, we have for the fourth summand that $\sum_i A(X_i)^2 = -\|A\|^2$. □

Recall from Definition 1.14 that $\tilde{a} \coloneqq 2\pi i a$.

Definition 1.36. A *potential* is a real-valued function $Q \in C^\infty(M)$. For $a \in \mathbb{R}^{n\prime}$ let $\Delta_a^{\mathrm{D}} + Q$ denote the *Schrödinger operator* and define the *spectrum* $\mathrm{Spec}_a(Q, \omega)$ of the translation-invariant connection $\nabla^{\mathrm{D}} + \tilde{a}$ on ω and the potential Q as the set of eigenvalues with multiplicities of the Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$ acting on smooth sections $\mathcal{E}(\omega)$ of the line bundle ω. Here, an eigenvalue λ is a complex number with the property that there is a nonvanishing eigensection $s \in \mathcal{E}(\omega)$ with $(\Delta_a^{\mathrm{D}} + Q)s = \lambda s$.

The map that assigns the spectrum of the corresponding Schrödinger operator to each translation-invariant connection

$$\mathbb{R}^{n\prime}/\mathcal{L}' \ni [a] \mapsto \mathrm{Spec}_a(Q, \omega)\,,$$

is called the *ω-Bloch spectrum* of Q.

Remark 1.37. The ω-Bloch spectrum is indeed well-defined because Hermitian translation-invariant connections differing by an element of $\mathcal{L}'$ are gauge equivalent and gauge equivalent connections on ω have the same spectrum: If we are given two connections intertwined by an ω-automorphism Φ, $\nabla_1 \circ \Phi = \Phi \circ \nabla_2$, and an eigenvalue $\lambda \in \mathbb{C}$ of the Schrödinger operator belonging to ∇_2 with eigensection $s \in \mathcal{E}(\omega)$, $(\Delta_2 + Q)s = \lambda s$, then $A \circ s$ is an eigensection with eigenvalue λ of the Schrödinger operator belonging to ∇_1.

Remark 1.38. Every Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$ is symmetric with respect to the inner products $\langle\,.\,,.\,\rangle_{\mathrm{L}^2}$ of ω because every connection $\nabla^{\mathrm{D}} + \tilde{a}$ is Hermitian and every potential Q is real-valued. Therefore, every eigenvalue λ is actually a real number.

The ω-Bloch spectrum contains the spectra of all translation-invariant connections since gauge equivalent connections have the same spectrum.

Remark 1.39 (Classical Bloch spectrum).
For every $a \in \mathbb{R}^{n\prime}$ and every potential Q on M the spectrum $\mathrm{Spec}_a(Q, \omega)$ coincides with the spectrum of the operator $\Delta_0^{\mathrm{D}} + Q$ acting on the space of all smooth sections $s \in \mathcal{E}(\theta^1)$ of the trivial bundle θ^1 over $\mathbb{R}^n$ satisfying

$$s(x + l) = \mathrm{e}^{\tilde{a}(l)} e_l(x) s(x) \qquad \text{for all } x \in M \text{ and } l \in \mathcal{L}.$$

To see this, observe that the bundle automorphism

$$\theta^1 \ni (x, z) \mapsto (x, \mathrm{e}^{\tilde{a}(x)} z) \in \theta^1$$

maps the lifts of sections of ω to sections of θ^1 with the above property, and intertwines $\nabla^{\mathrm{D}} + \tilde{a}$ and $\nabla^{\mathrm{D}} + 0$ acting these spaces.

The Chern class of the trivial bundle $\pi\colon M\times\mathbb{C}\to M$ over M is 0 and thus its harmonic representative also vanishes. Hence, $F=0$ and, arguing analogously to the case with a nondegenerate F, $w_l=0$ for all $l\in\mathcal{L}$. The distinguished connection is given by $\nabla^{\mathrm{D}}=\mathrm{d}$ and the Laplacian is just the Euclidean Laplacian defined by the Euclidean metric. The spectrum $\mathrm{Spec}_a(Q)$ is the spectrum of the Schrödinger operator $\Delta+Q$ acting on smooth functions $f\in C^\infty(\mathbb{R}^n,\mathbb{C})$ with $f(x+l)=\mathrm{e}^{\tilde{a}(l)}f(x)$. Thus, the definition of the Bloch spectrum agrees in this case with the classical definition of the Bloch spectrum.

Chapter 2

Transplantations and Types

Both the positive and negative spectral results of this thesis rely on expressing the potentials Q as Fourier series. In this chapter we will first introduce some notation of the Fourier expansion and recall that the exponential functions $E_c = \mathrm{e}^{-\tilde{c}}$ with $c \in \mathcal{L}'$ form a Hilbert basis for the L^2-sections of ω.

The negative results of this work are found by constructing so-called transplantations between distinct yet isospectral objects.

Definition 2.1. Given two Hilbert spaces with two operators $D_1 \colon H_1 \to H_1$ and $D_2 \colon H_2 \to H_2$ such that D_1 has a spectral resolution $D_1\phi_i = \lambda_i\phi_i$ with $\{\phi_i\}$ spanning H_1, then a *transplantation* from D_1 to D_2 is an isomorphism

$$T \colon H_1 \to H_2$$

such that eigenvectors of D_1 are mapped to eigenvectors of D_2 with the same eigenvalue,

$$D_2(T\phi_i) = \lambda_i T\phi_i \,.$$

If there exists a transplantation between two operators they must be isospectral.

A linear map $T \colon H_1 \to H_2$ *intertwines* two operators, say two connections ∇^1 and ∇^2, if $\nabla^2 \circ T = T \circ \nabla^1$. An intertwining map gives rise to a transplantation of the corresponding Laplacians.

Writing the potential Q as a Fourier series we will construct, under certain conditions, transplantations between the Schrödinger operators $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b^{\mathrm{D}} + Q$ induced by different translation-invariant connections $a, b \in \mathbb{R}^{n'}$ for some fixed potential Q. We will show that the constructed maps are indeed transplantations by proving that they intertwine the corresponding Schrödinger operators.

For such transplantations to exist we require that the potential and the involved connections satisfy either of two conditions with respect to the curvature form $-\tilde{F}$. We will introduce a new name for triples (Q, a, b) that satisfy these conditions: We say that they are of type (M) or of type (P), see Definition 2.13. We will also provide an alternative description of these types and we will construct an example for which the connections a and b are isospectral even if the triples (Q, a, b) is of mixed type.

In Chapter 6 we will use the wave invariants to show that at least under certain assumptions the converse of these statements is also true: If a and b are isospectral then they must be of a certain type with respect to Q.

It should be noted that while we do use the map $\check{x} := -x$ from [GGKW08, Definition 2.12], the transplantations given here and the definition of types was not contained in [GGKW08] nor [Ber17]. In those works the focus was primarily on results regarding the extent to which a potential Q is determined by the spectrum of some connection or set of connections. Here we ask the converse question: To what extent is a connection determined by the spectrum of a fixed potential?

Now, let us start with a reminder of Fourier series and some related notations that will be used throughout this thesis. We continue to write $\tilde{c} = 2\pi i c$ as in Definition 1.14.

Definition 2.2. On the smooth functions $C^\infty(M, \mathbb{C})$ of a flat torus $M = \mathbb{R}^n/\mathcal{L}$ given by some lattice $\mathcal{L}$ we define an inner product

$$\langle f, g\rangle := \tfrac{1}{\operatorname{Vol} M} \int_M f \cdot \overline{g}\, \mathrm{d}V\,.$$

$\mathrm{L}^2(M)$ is the completion of $C^\infty(M, \mathbb{C})$ with respect to this product. Given a dual lattice vector $c \in \mathcal{L}'$ define a smooth complex-valued function

$$E_c \colon M \to \mathbb{C} \qquad \text{by} \qquad E_c := \mathrm{e}^{-\tilde{c}}\,.$$

Given some L^2-function f on M denote the Fourier coefficients of f by

$$f_c := \langle f, E_c\rangle\,.$$

The *frequency support* of some function $f \in \mathrm{L}^2(M)$ is the set of dual lattice vectors with nonzero Fourier coefficients,

$$\mathcal{L}'_f := \{c \in \mathcal{L}' \mid f_c \neq 0\} \subset \mathcal{L}'\,.$$

The following Theorem is well-known. A proof can be found in [Gra08].

Theorem 2.3. The functions $\{E_c\}_{c\in\mathcal{L}'}$ form a Hilbert basis for the Hilbert space $(\mathrm{L}^2(M), \langle\,.\,,.\,\rangle)$ for all flat tori $M = \mathbb{R}^n/\mathcal{L}$, i.e.

$$f = \sum_{c\in\mathcal{L}'} f_c E_c \qquad \text{in the } \mathrm{L}^2\text{-sense for all } f \in \mathrm{L}^2(M).$$

Lemma 2.4. A function $Q \in \mathrm{L}^2(M)$ is real-valued if and only if $Q_{-c} = \overline{Q_c}$ for all $c \in \mathcal{L}'_Q$. In particular,

$$c \in \mathcal{L}'_Q \quad \Leftrightarrow \quad -c \in \mathcal{L}'_Q\,.$$

With $\check{Q}(x) \coloneqq Q(-x)$ as in Definition 1.25 we call Q *even* if $\check{Q} = Q$ and *odd* if $\check{Q} = -Q$. Q is an even function if and only if the imaginary part $\operatorname{Im} Q_c$ is zero for all $c \in \mathcal{L}'$. Q is an odd function if and only if $\operatorname{Re} Q_c = 0$ for all $c \in \mathcal{L}'$.

Proof. If Q is real-valued then $\overline{Q} = Q$ and

$$\overline{Q_c} = \overline{\langle Q, E_c\rangle} = \langle \overline{Q}, \overline{E_c}\rangle = \langle Q, E_{-c}\rangle = Q_{-c}\,.$$

If on the other hand $Q_{-c} = \overline{Q_c}$ then

$$\overline{Q} = \sum_{c\in\mathcal{L}'_Q} \overline{Q_c E_c} = \sum_{c\in\mathcal{L}'_Q} Q_{-c}E_{-c} = Q$$

and Q must be real-valued.

The connection between the parity of Q and its Fourier coefficients is obtained by comparing the Fourier coefficients in the following two series.

$$\sum_{c\in\mathcal{L}'} Q_c E_c = Q = \pm\check{Q} = \pm\sum_{c\in\mathcal{L}'} Q_c E_{-c} = \sum_{c\in\mathcal{L}'} \pm Q_{-c}E_c = \sum_{c\in\mathcal{L}'} \pm\overline{Q_c}E_c\,. \qquad \square$$

It follows from this Lemma that every Q_c with $c \in \mathcal{L}'$ gives rise to a real-valued smooth function Q on M if it decreases sufficiently fast for $c \to \infty$ and satisfies $Q_{-c} = \overline{Q_c}$.

With the Fourier series as a tool at hand we can proceed to construct transplantations between the connections a and b.

Definition 2.5. For any alternating bilinear form $F\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ we define a map

$$\mathbb{R}^n \ni X \mapsto F(X,\,.\,) \in \mathbb{R}^{n\prime}$$

that is also denoted by F, so $FX \coloneqq F(X,\,.\,)$. If F is nondegenerate then denote the inverse of this function by G:

$$G \coloneqq F^{-1}\colon \mathbb{R}^{n\prime} \to \mathbb{R}^n\,.$$

With the notation of Definition 1.9 we have the following.

Lemma 2.6. For all $X \in \mathbb{R}^n$ and $a \in \mathbb{R}^{n\prime}$

$$w_{Ga}(X) = a(\mathrm{pr}_{\mathfrak{V}} X) \qquad \text{and} \qquad w_X(Ga) = -a(\mathrm{pr}_{\mathfrak{U}} X)\,,$$

where $\mathrm{pr}_{\mathfrak{U}}$ and $\mathrm{pr}_{\mathfrak{V}}$ are the projections on the linear span of $\mathfrak{U} := \{U_i\}$ and $\mathfrak{V} := \{V_i\}$.

Proof. Writing $a = a_i^U U^i + a_i^V V^i$ and $X = x_U^i U_i + x_V^i V_i$ we have

$$\begin{aligned} w_{Ga}(X) &= \sum r_i u^i(Ga) v^i(X) \\ &= \sum r_i u^i(-a_j^U V_j/r_j + a_j^V U_j/r_j) v^i(X) = a_i^V x_V^i = a(\mathrm{pr}_{\mathfrak{V}} X)\,. \end{aligned}$$

The second claim follows analogously. □

We write $E_h := \mathrm{e}^{-\tilde{h}}$, analogously to the case of dual lattice vectors c.

Lemma 2.7 (Ψ_h).
For all $a, h \in \mathbb{R}^{n\prime}$ the map

$$\begin{aligned} &\Psi_h \colon C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \to C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \qquad \text{defined by} \\ &\Psi_h f := (E_h \circ \mathrm{pr}_{\mathfrak{U}}) \cdot f(\,.\, - Gh) \end{aligned}$$

is a well-defined isometric isomorphism and intertwines ∇^{a-h} and ∇^a, explicitly $\Psi_h \circ \nabla^{a-h} = \nabla^a \circ \Psi_h$.

Proof. Ψ_h is well-defined if $\Psi_h f(x+l) = e_l(x)\Psi_h f(x)$ for all $x \in \mathbb{R}^n$, $l \in \mathcal{L}$ and any smooth function with $f(x+l) = e_l(x) f(x)$. This is indeed the case:

$$\begin{aligned} \Psi_h f(x+l) &= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x+l) \cdot f(x - Gh + l) = E_h \circ \mathrm{pr}_{\mathfrak{U}}(l) \cdot e_l(x - Gh) \cdot \Psi_h f(x) \\ &= \exp\Big(2\pi\mathrm{i}\big(-h(\mathrm{pr}_{\mathfrak{U}} l) + w_l(-Gh)\big)\Big) \cdot e_l(x)\Psi_h f(x) = e_l(x)\Psi_h f(x) \end{aligned}$$

since $w_l(Gh) = -h(\mathrm{pr}_{\mathfrak{U}} l)$ by Lemma 2.6.

The map Ψ_h is isometric in the sense that obviously

$$\langle \Psi_h f, \Psi_h g\rangle_{\mathrm{L}^2} = \langle f, g\rangle_{\mathrm{L}^2}\,.$$

To see that Ψ_h is an isomorphism note that Ψ_{-h} is its inverse up to a nonvanishing multiplicative constant:

$$\begin{aligned} \Psi_h \circ \Psi_{-h}(f) &= \Psi_h\Big(E_{-h} \circ \mathrm{pr}_{\mathfrak{U}} \cdot f(\,.\, + Gh)\Big) \\ &= E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot E_{-h} \circ \mathrm{pr}_{\mathfrak{U}}(\,.\, - Gh) \cdot f(\,.\, - Gh + Gh) = E_{-h} \circ \mathrm{pr}_{\mathfrak{U}}(-Gh) \cdot f \end{aligned}$$

Finally, for any $X \in \mathcal{X}(M)$ we have

$$\begin{aligned}
&\nabla^a_X(\Psi_h f) = X(\Psi_h f) + (A^{\mathrm{D}} + \tilde{a})(X) \cdot \Psi_h f \\
&= E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \Big(-\tilde{h}(\mathrm{pr}_{\mathfrak{U}}(X)) \cdot f(\,.\,- Gh) + (Xf)(\,.\,- Gh)\Big) \\
&\qquad + E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \Big(A^{\mathrm{D}}_{\,.\,-Gh+Gh}(X) + \tilde{a}(X)\Big) \cdot f(\,.\,- Gh) \\
&= \Psi_h\Big(Xf + (A^{\mathrm{D}}_{\,.\,+Gh}(X) + (-\tilde{h}(\mathrm{pr}_{\mathfrak{U}}(X)) + \tilde{a}(X)))f\Big) \\
&\qquad\qquad = \Psi_h\Big(\nabla^{a-h}_X f + (-(\tilde{a} - \tilde{h}) - \tilde{w}_{Gh} - \tilde{h} \circ \mathrm{pr}_{\mathfrak{U}} + \tilde{a})(X)\Big) = \Psi_h(\nabla^{a-h}_X f)
\end{aligned}$$

since $w_{Gh} = h \circ \mathrm{pr}_{\mathfrak{V}}$ again by Lemma 2.6. □

Corollary 2.8. Since Ψ_{a-b} intertwines ∇^b and ∇^a we have for vanishing potentials $Q = 0$ that

$$\mathrm{Spec}_a(0, \omega) = \mathrm{Spec}_b(0, \omega)$$

for all pairs $a, b \in \mathbb{R}^{n\prime}$. That is Δ^{D}_a and Δ^{D}_b are always isospectral.

This corollary was already given in [Ber17, Corollary 7.1], [GKSW12, Lemma 3.1] and [GGKW08, Corollary 3.7].

If $Q \neq 0$ then Ψ_{a-b} is not necessarily a transplantation between $\Delta^{\mathrm{D}}_b + Q$ and $\Delta^{\mathrm{D}}_a + Q$. In Chapter 6 we will use the wave invariants to show the existence of potentials Q and connections a, b such that $\Delta^{\mathrm{D}}_a + Q$ and $\Delta^{\mathrm{D}}_b + Q$ are nonisospectral. If, however, the connections satisfy a condition on the frequency support of the potential then Ψ_{a-b} is a transplantation between the corresponding Schrödinger operators.

Lemma 2.9. If for all $c \in \mathcal{L}'_Q$ we have $E_c(G(a-b)) = 1$ then Ψ_{a-b} is a transplantation between $\Delta^{\mathrm{D}}_a + Q$ and $\Delta^{\mathrm{D}}_b + Q$. Thus,

$$\forall c \in \mathcal{L}'_Q : E_c(G(a-b)) = 1 \quad \Rightarrow \quad \mathrm{Spec}_a(Q, \omega) = \mathrm{Spec}_b(Q, \omega)\,.$$

Proof. The assumption implies $Q = \sum_{c \in \mathcal{L}'_Q} Q_c E_c = \sum_{c \in \mathcal{L}'_Q} Q_c E_c(\,.\,- G(a-b)) = Q(\,.\,- G(a-b))$ and thus, for all $f \in C^\infty(M, \mathbb{C})^{\mathcal{L}} \cong \mathcal{E}(\omega)$:

$$\begin{aligned}
\Psi_{a-b}(Qf) &= E_{a-b} \circ \mathrm{pr}_{\mathfrak{U}} \cdot Q(\,.\,- G(a-b)) f(\,.\,- G(a-b)) \\
&\qquad = Q \cdot E_{a-b} \circ \mathrm{pr}_{\mathfrak{U}} \cdot f(\,.\,- G(a-b)) = Q \cdot \Psi_{a-b} f\,.
\end{aligned}$$

In other words, Ψ_{a-b} does not only intertwine ∇^b and ∇^a but also the multiplication operator $f \mapsto Q \cdot f$ with itself. Therefore, Ψ_{a-b} is a transplantation from $\Delta^{\mathrm{D}}_b + Q$ to $\Delta^{\mathrm{D}}_a + Q$ and those two operators must hence be isospectral. □

Lemma 2.9 gives us a sufficient condition for the isospectrality of connections given some potential. The following Lemma together with Lemma 2.12 give us a second such condition.

Lemma 2.10 (Φ_h).
For all $a, h \in \mathbb{R}^{n\prime}$ the map

$$\Phi_h \colon C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \to C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \qquad \text{defined by}$$
$$\Phi_h f \coloneqq E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \check{f}(\,.\, - Gh)$$

is a well-defined isometric isomorphism and intertwines ∇^{h-a}_{-X} and ∇^a_X, explicitly $\Phi_h \circ \nabla^{h-a}_{-X} = \nabla^a_X \circ \Phi_h$. Since $\{-X_i\}$ is an orthonormal frame if $\{X_i\}$ is one, Φ_h intertwines $\Delta^{\mathrm{D}}_{h-a}$ with Δ^{D}_a.

Proof. Φ_h is well-defined if $\Phi_h f(x+l) = e_l(x)\Phi_h f(x)$ for all $x \in \mathbb{R}^n, l \in \mathcal{L}$ and any smooth function with $f(x+l) = e_l(x)f(x)$, this is indeed the case:

$$\begin{aligned}
\Phi_h f(x+l) &= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x+l) \cdot \check{f}(x - Gh + l) = E_h \circ \mathrm{pr}_{\mathfrak{U}}(x+l) \cdot f(-x + Gh - l) \\
&= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x+l) \cdot e_{-l}(-x+Gh) f(-x+Gh) = E_h \circ \mathrm{pr}_{\mathfrak{U}}(l) \cdot e_l(x - Gh)\Phi_h f(x) \\
&= \exp 2\pi\mathrm{i}(-h(\mathrm{pr}_{\mathfrak{U}} l) - w_l(Gh)) \cdot e_l(x)\Phi_h f(x) = e_l(x)\Phi_h f(x)\,,
\end{aligned}$$

by Lemma 2.6. It is obvious that Φ_h is an isometry:

$$\langle \Phi_h f, \Phi_h g \rangle_{\mathrm{L}^2} = \langle f, g \rangle_{\mathrm{L}^2}\,.$$

To see that Φ_h is an isomorphism note that Φ_h is its own inverse up to a nonvanishing multiplicative constant:

$$\begin{aligned}
&\Phi_h \circ \Phi_h(f)(x) = \Phi_h\Big(E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \check{f}(\,.\, - Gh)\Big)(x) \\
&= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x) \cdot \Big(E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \check{f}(\,.\, - Gh)\Big)\check{}\,(x - Gh) \\
&= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x) \cdot \Big(E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \check{f}(\,.\, - Gh)\Big)(-x + Gh) \\
&\qquad = E_h \circ \mathrm{pr}_{\mathfrak{U}}(x) \cdot E_h \circ \mathrm{pr}_{\mathfrak{U}}(-x + Gh) \cdot \check{f}(-x) = E_h \circ \mathrm{pr}_{\mathfrak{U}}(Gh) \cdot f(x)\,.
\end{aligned}$$

Further, we have for any translation-invariant vector field $X \in \mathcal{X}(M)$ that

$$\begin{aligned}
&\nabla^a_X \Phi_h f(x) = X_x(\Phi_h f) + \Big(A^{\mathrm{D}}_x(X) + \tilde{a}(X)\Big) \cdot \Phi_h f(x) \\
&= X_x\Big(E_h(\mathrm{pr}_{\mathfrak{U}})\check{f}(\,.\, - Gh)\Big) + \Big(A^{\mathrm{D}}_x(X) + \tilde{a}(X)\Big) \cdot \Phi_h f(x) \\
&= E_h(\mathrm{pr}_{\mathfrak{U}} x) \cdot \Big(- \tilde{h}(\mathrm{pr}_{\mathfrak{U}} X) f(-x + Gh) - X_{-x+Gh} f \\
&\qquad\qquad + \Big(A^{\mathrm{D}}{}_{-x+Gh-Gh}(-X) - \tilde{a}(-X)\Big) \cdot f(-x + Gh)\Big) \\
&= \Phi_h\Big(-Xf + A^{\mathrm{D}}(-X)f + \Big(\tilde{h} \circ \mathrm{pr}_{\mathfrak{U}} - \tilde{a} + \tilde{w}_{Gh}\Big)(-X)f\Big)(x) \\
&= \Phi_h\Big(-Xf + A^{\mathrm{D}}(-X)f + \Big(\tilde{h} \circ \mathrm{pr}_{\mathfrak{U}} - \tilde{a} + \tilde{h} \circ \mathrm{pr}_{\mathfrak{V}}\Big)(-X)f\Big)(x) = \Phi_h\Big(\nabla^{h-a}_{-X}\Big)
\end{aligned}$$

by Lemma 2.6. □

As was the case for Lemma 2.7 and Corollary 2.8 we can again conclude that for vanishing potentials the Laplacians are all isospectral.

Corollary 2.11. Since Φ_{a+b} intertwines Δ_a^{D} and Δ_b^{D} we have for vanishing potentials $Q = 0$ that

$$\mathrm{Spec}_a(0,\omega) = \mathrm{Spec}_b(0,\omega)$$

for all pairs $a, b \in \mathbb{R}^{n\prime}$. That is Δ_a^{D} and Δ_b^{D} are isospectral.

Just as before this does not generalize to all potentials. For $Q \neq 0$ the map Φ_{a+b} does not, in general, need to be a transplantation from $\Delta_a^{\mathrm{D}} + Q$ to $\Delta_b^{\mathrm{D}} + Q$.

Lemma 2.12. If we have for a potential Q on M that

$$\forall_{c\in\mathcal{L}'_Q} : Q_c = \overline{Q_c} \cdot E_{-c} \circ G(a+b)$$

then Φ_{a+b} is a transplantation between $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b^{\mathrm{D}} + Q$ and

$$\mathrm{Spec}_a(Q,\omega) = \mathrm{Spec}_b(Q,\omega)\,.$$

Proof. With $h \coloneqq a + b$ we have that Φ_h is a transplantation if $\Phi_h(Qf) = Q \cdot \Phi_h f$, which is the case if

$$\sum_{c\in\mathcal{L}'_Q} Q_c E_c(x) = Q(x) = \check{Q}(x - Gh) = \sum_{c\in\mathcal{L}'_Q} Q_c E_c(-x + Gh) = \sum_{c\in\mathcal{L}'_Q} Q_{-c} E_c(x - Gh)\,.$$

This is equivalent to

$$\forall_{c\in\mathcal{L}'_Q} : Q_c = Q_{-c} E_c(-Gh) = \overline{Q_c} E_{-c} \circ G(a+b)\,. \qquad \square$$

We now define the types of triples (Q,a,b) and use this concept to condense the results of this section into the following theorem.

Definition 2.13. A triple $(Q,a,b) \in C^\infty(M) \times \mathbb{R}^{n\prime} \times \mathbb{R}^{n\prime}$ consisting of a potential and two translation-invariant connections is said to be

- of *type (M)* with respect to $c \in \mathcal{L}'_Q$ if $E_c \circ G(a-b) = 1$ and
- of *type (P)* with respect to $c \in \mathcal{L}'_Q$ if $Q_c = \overline{Q_c} \cdot E_{-c} \circ G(a+b)$.

If (Q,a,b) is of type (M) or of type (P) if it is of this same type for all $c \in \mathcal{L}'_Q$. If the triple is of either but not necessarily the same type for all $c \in \mathcal{L}'_Q$ then (Q,a,b) is of *mixed type*.

Theorem 2.14. If Q is a smooth potential on a flat torus M and two translation-invariant connections on a nondegenerate line bundle ω are given by $a, b \in \mathbb{R}^{n\prime}$ such that (Q, a, b) is of type (M) or of type (P) then $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b^{\mathrm{D}} + Q$ are isospectral,

$$\mathrm{Spec}_a(Q, \omega) = \mathrm{Spec}_b(Q, \omega)\,.$$

Corollary 2.15. If $Q \equiv Q_0 \in \mathbb{R}$ is constant then (Q, a, b) is of type (M) and of type (P) for all $a, b \in \mathbb{R}^{n\prime}$. In particular, as we saw already in Corollary 2.8, all connections are isospectral.

Note that the type of dual lattice vectors c and $-c$ agree: If (Q, a, b) is of one of the two types with respect to c then it also of the same type with respect to $-c$.

Theorem 2.14 is applicable only if the triple (Q, a, b) is of type (M) or (P) but the types are not mixed. If (Q, a, b) is of mixed type we cannot, in general, conclude that the corresponding Schrödinger operators are isospectral. However, in the remainder of this section we will give an example that shows that for some special lattices $\mathcal{L}$ and potentials Q it is possible to combine the transplantations Ψ and Φ of Lemma 2.7 and 2.10 to obtain a transplantation even though (Q, a, b) is only of mixed type.

But first, the definition of the two types can be reformulated as follows.

Remark 2.16. For a nondegenerate alternating bilinear form $F\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ we can define an alternating bilinear form on the dual space by

$$F'(a, b) \coloneqq F(Ga, Gb) \qquad \text{for } a, b \in \mathbb{R}^{n\prime},$$

where G is the inverse of F as in Definition 2.5. If $\{U_i, V_i\}$ is a Chern basis for F with Chern factors $r_i \in \mathbb{Z}$ then the dual basis $\{U^i, V^i\}$ satisfies

$$F'(U^i, V^i) = F(GU^i, GV^i) = F(-V_i/r_i, U_i/r_i) = \frac{F(U_i, V_i)}{r_i^2} = \frac{1}{r_i}\,.$$

In particular, $F'(\mathcal{L}', \mathcal{L}') \not\subset \mathbb{Z}$ if $r_{n/2} \neq 1$. Further note that $\{U_i/r_i, V_i\}$ is a Darboux basis for F and the corresponding dual basis $\{r_i U^i, V^i\}$ satisfies

$$F'(r_i U^i, V^i) = 1\,.$$

It is therefore a Darboux basis for F'.

Let $[.]$ denote classes in $\mathbb{R}/\mathbb{Z}$ and write the Fourier coefficients Q_c in polar form as

$$Q_c = q_c \mathrm{e}^{2\pi \mathrm{i} \phi_c(Q)} \qquad \text{with } q_c \geq 0 \text{ and } 0 \leq \phi_c < 1.$$

Then the triple $(Q, a, b) \in C^\infty(M) \times \mathbb{R}^{n'} \times \mathbb{R}^{n'}$ is

– of *type (M)* exactly if $[F'(c, a-b)] = 0$ for all $c \in \mathcal{L}'_Q$ and

– of *type (P)* exactly if $[F'(c, a+b)] = [2\phi_c(Q)]$ for all $c \in \mathcal{L}'_Q$.

The first claim follows from $F'(c, a-b) = F(Gc, G(a-b)) = c(G(a-b))$. Thus, $[F'(c, a-b)] = 0$ is equivalent to $E_c \circ G(a-b) = 1$.

Since Q is real-valued we must have $\phi_{-c}(Q) = -\phi_c(Q)$ and therefore (Q, a, b) is of type (P) with respect to c exactly if

$$(\mathrm{e}^{2\pi \mathrm{i} \phi_c(Q)})^2 = E_{-c} \circ G(a+b) \qquad \text{or equivalently}$$
$$[2\phi_c(Q)] = [c \circ G(a+b)] = [F(Gc, G(a+b))] = [F'(c, a+b)]$$

for all $c \in \mathcal{L}'_Q$. The conditions of both types are tested only on those dual lattice vectors $c \in \mathcal{L}'$ which lie in the frequency support of the potential Q. Apart from that, the condition of type (M) does not refer to the potential Q and the condition of type (P) depends only on the phases but not the absolute values of the Fourier coefficients.

In the following Lemma we write for any set $I \subset \{1, \dots, n/2\}$

$$\mathbb{Z}(U^I, V^I) \coloneqq \mathrm{Span}_{\mathbb{Z}} \left\{ U^i, V^i \mid i \in I \right\}.$$

Lemma 2.17. Consider an even-dimensional lattice $\mathcal{L} \coloneqq \mathbb{Z}(U_i, V_i)$, where the Chern basis vectors are proportional to the standard basis. Let Q be a potential with frequency support $\mathcal{L}'_Q \subset \mathbb{Z}(U^I, V^I) \cup \mathbb{Z}(U^J, V^J)$, where $I \cup J = \{1, \dots, n/2\}$ are two disjoint sets. Further assume that (Q, a, b) is of type (M) with respect to the frequencies in $\mathbb{Z}(U^I, V^I)$ and of type (P) with respect to the frequencies in $\mathbb{Z}(U^J, V^J)$. Even though (Q, a, b) is only of mixed type there exists a transplantation which intertwines $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b^{\mathrm{D}} + Q$. In particular, a and b are isospectral with respect to Q.

Proof. By assumption, $U_i = C_i \cdot e_i$ and $V_i = C_{i+n/2} \cdot e_{i+n/2}$ for some $C_k \in \mathbb{R}$. For any $x \in \mathbb{R}^n$ define $\hat{x}$ by setting $\hat{x}_i \coloneqq x_i$ for $i \in I \cup (I + n/2)$ and $\hat{x}_j \coloneqq -x_j$ for $j \in J \cup (J + n/2)$. For a function f on $\mathbb{R}^n$ set $\hat{f}(x) \coloneqq f(\hat{x})$. For $h \in \mathbb{R}^{n'}$ define

$$\Lambda_h f \coloneqq E_h \circ \mathrm{pr}_{\mathfrak{U}} \cdot \hat{f}(\,. - Gh)\,.$$

This is well-defined map $\Lambda_h \colon C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}} \to C^\infty(\mathbb{R}^n, \mathbb{C})^{\mathcal{L}}$ because for $l \in \mathcal{L}$

$$\Lambda_h f(x + l) = E_h \circ \mathrm{pr}_{\mathfrak{U}}(x + l) \hat{f}(x + l - Gh) =$$
$$= E_h \circ \mathrm{pr}_{\mathfrak{U}}(x + l) \cdot f(\hat{x} - (Gh)\hat{}) \cdot e_{\hat{l}}(\hat{x} - (Gh)\hat{}) = e_l(x) \Lambda_h f(x)$$

as $e_{\hat{l}}(\hat{x}) = e_l(x)$ and $E_h \circ \mathrm{pr}_{\mathfrak{U}}(l) \cdot e_{\hat{l}}(-(Gh)\hat{}) = 1$. Further, Λ_h clearly preserves the L^2-norm and it is surjective because $\Lambda_{-\hat{h}}$ is an inverse up to a multiplicative constant of norm 1.

A calculation similar to the proofs of Lemmas 2.7 and 2.10 shows that

$$\begin{aligned}
&\nabla^a_{e_i}\Lambda_h f = \Lambda_h \nabla^{a-h}_{e_i} f && \text{for } i \in I \cup (I + n/2) \text{ and}\\
&\nabla^a_{e_j}\Lambda_h f = \Lambda_h \nabla^{-a+h}_{-e_j} f && \text{for } j \in J \cup (J + n/2).
\end{aligned}$$

Note that $\hat{b}(e_i) = b(e_i)$, $\nabla^{\hat{b}}_{e_i} = \nabla^b_{e_i}$ and $\hat{b}(e_j) = -b(e_j)$, $\nabla^{-\hat{b}}_{-e_j} = \nabla^b_{-e_j}$. It follows that

$$\begin{aligned}
&\nabla^a_{e_i} \circ \nabla^a_{e_i} \circ \Lambda_{a-\hat{b}} = \Lambda_{a-\hat{b}} \circ \nabla^{a-a+\hat{b}}_{e_i} \circ \nabla^{a-a+\hat{b}}_{e_i} = \Lambda_{a-\hat{b}} \circ \nabla^b_{e_i} \circ \nabla^b_{e_i} && \text{and}\\
&\nabla^a_{e_j} \circ \nabla^a_{e_j} \circ \Lambda_{a-\hat{b}} = \Lambda_{a-\hat{b}} \circ \nabla^{-a+a-\hat{b}}_{-e_j} \circ \nabla^{-a+a-\hat{b}}_{-e_j} = \Lambda_{a-\hat{b}} \circ \nabla^b_{e_j} \circ \nabla^b_{e_j}
\end{aligned}$$

Thus, $\Lambda_{a-\hat{b}}$ intertwines the two Laplace operators Δ^{D}_b and Δ^{D}_a.

It remains to show that $\Lambda_{a-\hat{b}}$ also intertwines the operator $f \mapsto Q \cdot f$. By assumption we can split the frequency support $\mathcal{L}'_Q = \mathcal{L}'_- \cup \mathcal{L}'_+$ into one part, $\mathcal{L}'_-$, corresponding to I and one, $\mathcal{L}'_+$, corresponding to J. This split is chosen such that (Q, a, b) is of type (M) for the elements of $\mathcal{L}'_-$ and of type (P) for $\mathcal{L}'_+$. Thus, for $c \in \mathcal{L}'_-$, $\hat{E}_c = E_c$ and hence

$$\hat{E}_c(-G(a-\hat{b})) = E_c(-G(a-b)) = 1;$$

for $c \in \mathcal{L}'_+$, $\hat{E}_c(h) = E_c(-h)$ for all $h \in \mathbb{R}^n$ and thus

$$Q_c \hat{E}_c(-G(a-\hat{b})) = Q_c E_c(G(a+b)) = Q_{-c}\,.$$

Therefore,

$$\begin{aligned}
&\Lambda_{a-\hat{b}}(Q \cdot f) = \hat{Q}(\,.\,- G(a-\hat{b})) \cdot \Lambda_{a-\hat{b}} f\\
&= \Big(\sum_{c\in\mathcal{L}'_-} Q_c \hat{E}_c \cdot \hat{E}_c(-G(a-\hat{b})) + \sum_{c\in\mathcal{L}'_+} Q_c \hat{E}_c \cdot \hat{E}_c(-G(a-\hat{b}))\Big) \cdot \Lambda_{a-\hat{b}} f\\
&\qquad = \Big(\sum_{c\in\mathcal{L}'_-} Q_c E_c + \sum_{c\in\mathcal{L}'_+} Q_{-c} E_{-c}\Big) \cdot \Lambda_{a-\hat{b}} f = Q \cdot \Lambda_{a-\hat{b}} f\,.
\end{aligned}$$

This implies that $\Lambda_{a-\hat{b}}$ is a transplantation from $\Delta^{\mathrm{D}}_b + Q$ to $\Delta^{\mathrm{D}}_a + Q$. □

In [Ber17] I have constructed explicit transplantations using ideas presented in [GGKW08]. Those transplantations were constructed to find isospectrality relations among the Schrödinger operators given by differing potentials Q but fixed connections. The special case $Q = 0$ in [Ber17, Corollary 7.1] resulted in a transplantation similar to the transplantation Ψ of Lemma 2.7. Changing the focus by keeping the potential Q constant and varying the connections led to the construction of the new transplantations given here.

Chapter 3

Heat Invariants

The transplantations in the previous sections provide information as to what is *not* determined by the spectrum of the Schrödinger operators $\Delta_a^{\mathrm{D}} + Q$. To obtain converse results we need *spectral invariants* of which we will study two types: the *heat invariants* and the *wave invariants*.

The heat invariants of Laplace-type operators have been studied extensively by, for example, Peter Gilkey in [Gil75], [Gil78] and [Gil95]. Although the first four nontrivial heat invariants for general Laplace-type operators acting on sections of vector bundles on Riemannian manifolds are computed in [Gil95, Theorem 4.1.6] using functorial arguments we will calculate the heat invariants in our special case of flat tori directly using the computer algebra system MATHEMATICA. The MATHEMATICA notebook in Appendix C and [Ber18] will give an example of how to calculate invariants defined by some explicit formula; an example that is much simpler than in the case of wave invariants. This chapter presents the mathematical ideas behind the MATHEMATICA notebook.

Apart from serving as an introduction into the computation of invariants using MATHEMATICA we can also calculate higher invariants than given by Gilkey for the particular Schrödinger operators $\Delta_a^{\mathrm{D}} + Q$ under consideration here. In Theorem 5.8 we will construct so-called "small" wave invariants $\mathsf{wi}_{i,d}(a, Q)$ that can be shown to be spectral invariants for every nonzero length $d \in |\mathcal{L}|\backslash\{0\}$ of a lattice vector with the method presented in Chapters 4 and 5. This result can be extended to $d = 0$ using these higher heat invariants.

Further, we will see that the heat invariants do not depend upon the choice of translation-invariant connection $a \in \mathbb{R}^{n'}$, see notation 1.24, and can therefore give no spectral information about the connections.

3.1 General Principle

The aim of this section is to calculate the *Heat Invariants* of the Schrödinger operator $P \coloneqq \Delta_a^{\mathrm{D}} + Q$ with $Q \in C^\infty(M)$ a smooth function on M. We follow Gilkey's book [Gil95, Chapter 1.6 to 1.8]. The Laplacian stems from a translation-invariant connection $a \in \mathbb{R}^{n'}$, as in the previous two chapters. We continue to use the notation introduced there.

Since P is a symmetric elliptic partial differential operator on a compact manifold M without boundaries there exists by [Gil95, Lemma 1.6.3] a discrete spectral resolution $\{\phi_k, \lambda_k\}$ for P, i.e. $\{\phi_k\}$ is an orthonormal basis for $\mathrm{L}^2(\omega)$ and

$$P\phi_k = (\Delta_a^{\mathrm{D}} + Q)\phi_k = \lambda_k \phi_k \,.$$

We chose our scalar product $\langle \,.\,,\,. \,\rangle$ on $\mathrm{L}^2(M)$ with a normalization factor $1/\operatorname{Vol} M$ such that the functions $\{E_c \coloneqq \mathrm{e}^{-\tilde{c}}\}_{c\in\mathcal{L}'}$ form an orthonormal basis, see Definition 2.2. We define our scalar product on $\mathrm{L}^2(\omega)$ analogously.

Definition 3.1. With the Hermitian product $\langle \,.\,,\,. \,\rangle_{\omega_x}$ on the fiber ω_x we choose

$$\langle s_1, s_2\rangle_{\mathrm{L}^2(\omega)} \coloneqq \frac{1}{\operatorname{Vol} M} \int_M \langle s_1(x), s_2(x)\rangle_{\omega_x} \,\mathrm{d}x \qquad \text{for } s_1, s_2 \in \mathrm{L}^2(\omega)$$

as our scalar product on $\mathrm{L}^2(\omega)$.

Definition 3.2. Denote by $\mathcal{E}_t(\omega)$ the space of smooth "time-dependent" sections of ω, that is the space of sections $\mathbb{R}\times M \ni (t,x) \mapsto s(t,x) \in \omega$ that are smooth in any local trivialization.

For the partial differential operator P the *heat equation* is

$$(\partial_t + P)s(t,x) = 0 \qquad \text{and} \qquad \lim_{t\to 0} s(t,x) = s_0(x)$$

for $s \in \mathcal{E}_t(\omega)$ and with $t > 0$, $x \in M$ and $s_0 \in \mathcal{E}(\omega) \cong C^\infty(M,\mathbb{C})^{\mathcal{L}}$. With the discrete spectral resolution $\{\phi_k, \lambda_k\}$ the solution $\mathrm{e}^{-tP} f$ of the heat equation is given by the integral kernel

$$K(t,x,y) \coloneqq \sum_{k\in\mathbb{N}} \mathrm{e}^{-\lambda_k t} \phi_k(x) \otimes \phi_k^*(y) \in \operatorname{Hom}(\omega_y, \omega_x) \qquad \text{and}$$

$$\left(\mathrm{e}^{-tP} f\right)(x,t) = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} f_k \phi_k(x) = \frac{1}{\operatorname{Vol} M} \int_M K(t,x,y) f(y) \,\mathrm{d}y \,,$$

where the $f_k = \langle f, \phi_k\rangle_{\mathrm{L}^2}$ are the coefficients of f with respect to $\{\phi_k\}_{k\in\mathbb{N}}$ and ϕ_k^* are given by $\phi_k^*(f)(y) = \langle f, \phi_k\rangle_{\omega_y}$. Those sums converge and K is a smooth kernel function for the operator e^{-tP}.

Definition 3.3. The kernel K is called the *heat kernel* of P. The *heat trace* is defined as the trace of the operator e^{-tP}:

$$\mathrm{Tr}_{\mathrm{L}^2}(\mathrm{e}^{-tP}) \coloneqq \frac{1}{\mathrm{Vol}\, M} \int_M \mathrm{Tr}_{\omega_x} K(t,x,x)\, \mathrm{d}x\,.$$

The discussion above gives the following proposition.

Proposition 3.4. The heat trace satisfies

$$\mathrm{Tr}_{\mathrm{L}^2}(\mathrm{e}^{-tP}) = \frac{1}{\mathrm{Vol}\, M} \int_M \mathrm{Tr}_{\omega_x} K(t,x,x)\, \mathrm{d}x = \sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k}$$

and is therefore spectrally determined.

By [Gil95, Lemma 1.8.2] the heat kernel has an asymptotic expansion

$$K(t,x,x,P) \sim \sum_{k\in\mathbb{N}} e_k(x,P) t^{(k-n)/2} \qquad \text{for } t \to 0.$$

The goal of the remaining sections is to find a computable approximation to the heat kernel K from which we can derive the (unintegrated) heat invariants $e_k(x,P)$ of this asymptotic expansion.

The *symbolic spectrum* of Laplace-type operators P is the set

$$C(P) \coloneqq \{\lambda \in \mathbb{C} \mid \exists (x,\xi) \in \mathrm{T}^*M : \det(p_2(x,\xi) - \lambda) = 0\} = \mathbb{R}_{\geq 0} \subset \mathbb{C}\,,$$

where $p_2 \colon (x,\xi) \mapsto \|\xi\|^2 \cdot \mathrm{id}_{\omega_x}$ is the leading symbol of P. Let $\mathcal{R} \subset \mathbb{C}$ denote a region such that $C(P) \cap \mathcal{R} = \emptyset$ and such that the boundary γ of $\mathcal{R}$ is a continuous clockwise-oriented path consisting of a half-circle in the $\mathrm{Re}\,\lambda \leq 0$-plane and two rays in the $\mathrm{Re}\,\lambda \geq 0$-plane.

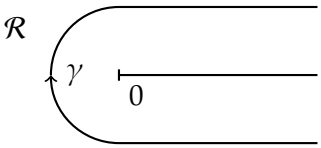


Figure 3.1: An exemplary choice of $\mathcal{R}$ and γ.

By [Gil95, Section 1.7.2 to 1.8] we have the following: For every sufficiently large $N \in \mathbb{N}$ and $\lambda \in \mathcal{R}$ one can construct operators $R_N(\lambda)$, which approximate $(P-\lambda)^{-1}$ in the sense that

$$(P-\lambda)R_N(\lambda) \sim_N \mathrm{id} \qquad \text{and} \qquad R_N(\lambda)(P-\lambda) \sim_N \mathrm{id}\,.$$

Here, $P \sim_N Q$ if $P - Q$ is a pseudo-differential operator of order $-N$. If one assumes that the half-circle within γ is sufficiently large one can use those

approximations to show that $P - \lambda$ is invertible and then the solution of the heat equation is given by the contour integral

$$e^{-tP} = \frac{1}{2\pi i} \int_\gamma e^{-t\lambda} (P - \lambda)^{-1} \lambda \, .$$

If N is sufficiently large, given some $k \in \mathbb{N}$, and $t > 0$ is small the operator

$$\frac{1}{2\pi i} \int_\gamma e^{-t\lambda} R_N(\lambda) \, d\lambda$$

has a smooth kernel K_N such that

$$\|K(t, x, y, P) - K_N(t, x, y, P)\|_{\infty,k} \leq C_k t^k \, .$$

From this it follows that the asymptotic expansions of the traces of both kernels are the same. In the next section we will explicitly calculate the asymptotic expansion of $K_N(t, x, x, P)$ for the Schrödinger operators under consideration.

3.2 Schrödinger operators

The symbols of the approximations $R_N(\lambda)$ will be given by an explicit combinatorial formula depending on the symbols of the operator $P = \Delta_a^D + Q$. As a first step, the symbols of P must be calculated.

Choose a fundamental domain U of the lattice and the standard coordinates x as a coordinate chart for M. Further, define the differential operators $D_x^\alpha := (-i)^{|\alpha|} \partial_x^\alpha$ for multiindices α.

With respect to the standard frame of TM induced by the trivial bundle over $\mathbb{R}^n$ we can calculate the Schrödinger operator P as in Proposition 1.35 and obtain

$$\Delta_a^D + Q = D_x^{2e_i} - 2iA_x(e_i) D_x^{e_i} - A_{e_i}^D(e_i) - A_x(e_i)^2 + Q$$

with the Einstein convention and $A = A^D + \tilde{a}$. Recall that $\operatorname{div}(A^\#) = e_i(A(e_i)) = A_{e_i}^D(e_i)$.

We could read off the symbols of P and proceed to compute the heat invariants. However, the local heat invariants do not depend on the choice of local frame, [Gil95, Lemma 1.8.2], and we can thus use the following, more convenient *a-frame* instead.

Definition 3.5. Define a smooth function $g \in C^\infty(U, \mathbb{C}\backslash\{0\})$ by

$$g(x) := e^{-\tilde{a}(x) - \frac{1}{2} A_x^D(x)} \, .$$

If s_1 is the standard local frame of ω induced by the standard frame of the trivial bundle, then define the *a-frame* by

$$s_2 := g \cdot s_1 \, .$$

Remark 3.6. In this a-frame the connection form of the connection a is given by half the curvature form $-\tilde{F}$ in the following sense: For all vector fields X on U we have

$$(Xg)(x) = g(x) \cdot \Big(-\tilde{a}(X_x) - \frac{1}{2}A^{\mathrm{D}}_{X_x}(x) - \frac{1}{2}A^{\mathrm{D}}_x(X_x)\Big).$$

Given any section $s = fs_2 = fgs_1$ with $f \in C^\infty(U)$ we have that

$$\begin{aligned}
&(\nabla^{\mathrm{D}} + \tilde{a})_X(s) = (X + A^{\mathrm{D}}(X) + \tilde{a}(X))(fgs_1) \\
&= X(f)gs_1 + fX(g)s_1 + (A^{\mathrm{D}} + \tilde{a})(X)fgs_1 \\
&= X(f)s_2 + f\Big(-\tilde{a}(X) - \frac{1}{2}A^{\mathrm{D}}_X - \frac{1}{2}A^{\mathrm{D}}(X)\Big)gs_1 + (A^{\mathrm{D}} + \tilde{a})(X)fs_2 \\
&\qquad = X(f)s_2 + f\Big(-\frac{1}{2}A^{\mathrm{D}}_X + \frac{1}{2}A^{\mathrm{D}}(X)\Big)s_2 = X(f)s_2 - \frac{1}{2}\tilde{F}(\,.\,, X)fs_2
\end{aligned}$$

by Lemma 1.15.

With respect to this a-frame the symbols of $\nabla^{\mathrm{D}} + \tilde{a}$ and therefore of $\Delta^{\mathrm{D}}_a + Q$ do not depend on the connection $a \in \mathbb{R}^{n'}$ but only on the curvature $-\tilde{F}$ of the translation-invariant connections. More explicitly, with respect to s_2 and with $\tilde{F}(e_i) \coloneqq \tilde{F}(e_i, \,.\,) = -\tilde{F}(\,.\,, e_i)$,

$$\begin{aligned}
&\Delta^{\mathrm{D}}_a + Q = -(\partial_{x_i} + \frac{1}{2}\tilde{F}(e_i))(\partial_{x_i} + \frac{1}{2}\tilde{F}(e_i)) + Q \\
&= -\partial^2_{x_i} - \frac{1}{2}\tilde{F}(e_i, e_i) - \tilde{F}(e_i)\partial_{x_i} - \frac{1}{4}\tilde{F}(e_i)^2 + Q \\
&\qquad\qquad = D^{2e_i}_x - \mathrm{i}\tilde{F}(e_i)D^{e_i}_x - \frac{1}{4}\tilde{F}(e_i)^2 + Q\,.
\end{aligned}$$

Therefore, the symbols of $P = \Delta^{\mathrm{D}}_a + Q$ are

$$\begin{aligned}
&p_2(x,\xi) = \xi_i^2 = \|\xi\|^2 \\
&p_1(x,\xi) = -\mathrm{i}\tilde{F}(e_i, x)\xi_i = -\mathrm{i}\tilde{F}(\xi, x) \qquad \text{and} \\
&p_0(x,\xi) = -\frac{1}{4}\tilde{F}(e_i, x)^2 + Q(x) = \frac{1}{4}\tilde{F}_2(x,x) + Q(x)\,,
\end{aligned}$$

where we use the following definition.

Definition 3.7 (Curvature traces).
For $X, Y \in \mathbb{R}^n$ and $k \in \mathbb{N}$ the *curvature traces* of F are recursively defined by

$$\begin{aligned}
&F_k(X,Y) \coloneqq \sum_{i=1}^{n} F_{k-1}(X, e_i)F(e_i, Y) \qquad \text{with} \\
&F_1(X,Y) \coloneqq F(X,Y)
\end{aligned}$$

and $\{e_i\}$ some orthonormal basis of $\mathbb{R}^n$. If such a curvature trace lacks arguments it is understood that one additional trace is computed:

$$F_k \coloneqq \operatorname{Tr} F_k(\,.\,,\,.\,)\,.$$

It is also understood that $\tilde{F}_k = (\tilde{F})_k = (2\pi\mathrm{i})^k F_k$.

Remark 3.8. The notation

$$F_k \coloneqq \operatorname{Tr} F_k(\,.\,,\,.\,) = F_k(e_i, e_i)$$

does not merely shorten expressions involved in computing heat and wave invariants by omitting the symbols e_i. This notation also allows MATHEMATICA to identify expressions that would need to be formally distinct when using indices. For example, MATHEMATICA does not "know" that

$$F_2(e_{i_1}, e_{i_1}) \cdot F_3(e_{i_2}, e_{i_2}) - F_2(e_{i_2}, e_{i_2}) \cdot F_3(e_{i_1}, e_{i_1}) = 0$$

but it does recognize that

$$F_2 \cdot F_3 - F_2 \cdot F_3 = 0\,.$$

Assigning different functions to the same symbol by using their *signature* is called *function overloading* in computer science.

Lemma 3.9. Curvature traces of odd order are antisymmetric, those of even order symmetric:

$$\tilde{F}_k(X, Y) = (-1)^k \tilde{F}_k(Y, X)\,.$$

Proof. Writing out the definition of the curvature traces and using the antisymmetry of F gives the result:

$$\begin{aligned}\tilde{F}_k(X, Y) &= \tilde{F}(X, e_{i_1})\tilde{F}(e_{i_1}, e_{i_2}) \cdots \tilde{F}(e_{i_{k-1}}, Y) \\ &= (-1)^k \tilde{F}(e_{i_1}, X)\tilde{F}(e_{i_2}, e_{i_1}) \cdots \tilde{F}(Y, e_{i_{k-1}}) \\ &= (-1)^k \tilde{F}(Y, e_{i_{k-1}}) \cdots \tilde{F}(e_{i_2}, e_{i_1})\tilde{F}(e_{i_1}, X) = (-1)^k \tilde{F}_k(Y, X)\end{aligned}$$ □

The heat invariants will be calculated from the symbols of the operator P with respect to the a-frame. Since those symbols do not depend on the connection a and since the heat invariants are invariantly defined, the heat invariants are independent of $a \in \mathbb{R}^{n\prime}$.

Now, set $\tilde{p}_0 \coloneqq p_0$, $\tilde{p}_1 \coloneqq p_1$ and

$$\tilde{p}_2(x, \xi, \lambda) \coloneqq p_2(x, \xi) - \lambda = \|\xi\|^2 - \lambda\,.$$

(We deviate from our definition of $\tilde{c} \coloneqq 2\pi\mathrm{i}c$ just once to stay in the notation of [Gil95].)

Let $S_2^h(\mathcal{R})$ denote the set of symbols with a complex parameter of order h as defined in [Gil95, Section 1.7.1]. We will now apply the general principle of Section 3.1 and construct the symbols of the operators $R_N(\lambda)$ such that

$$(P-\lambda)R_N(\lambda) \sim_N \mathrm{id} \qquad \text{and} \qquad R_N(\lambda)(P-\lambda) \sim_N \mathrm{id}$$

hold. As our ansatz we write the symbol of $R_N(\lambda)$ in local coordinates as

$$\sigma(R_N(\lambda)) = r_0 + \cdots + r_N \qquad \text{with } r_i \in S_2^{-2-i}(\mathcal{R})$$

and demand that

$$1 \overset{!}{\sim}_N \sigma((P-\lambda)R_N(\lambda)) \sim \sum_{\alpha,i,k} \partial_\xi^\alpha \tilde{p}_k \cdot D_x^\alpha r_i/\alpha!\,.$$

Since $\tilde{p}_k$ is a symbol of order k we have that $\partial_\xi^\alpha \tilde{p}_k \in S_2^{k-|\alpha|}(\mathcal{R})$ and $D_x^\alpha r_i \in S_2^{-2-i}(\mathcal{R})$, where 2 is the order of P. It follows that $\partial_\xi^\alpha \tilde{p}_k \cdot D_x^\alpha r_i/\alpha! \in S_2^{k-|\alpha|-i-2}(\mathcal{R})$. Comparing symbols of the same order h yields

$$1 \overset{!}{=} \sum_{0=k-|\alpha|-i-2} \partial_\xi^\alpha \tilde{p}_k \cdot D_x^\alpha r_i/\alpha! = \tilde{p}_2 \cdot r_0 \qquad \text{and}$$
$$0 \overset{!}{=} \sum_{-h=k-|\alpha|-i-2} \partial_\xi^\alpha \tilde{p}_k \cdot D_x^\alpha r_i/\alpha! = \tilde{p}_2 \cdot r_h + \sum_{h=|\alpha|+i+2-k,\, i<h} \partial_\xi^\alpha \tilde{p}_k \cdot D_x^\alpha r_i/\alpha!\,,$$

confer [Gil95, (1.7.29)]. Note that in the last sum $\partial_x^\alpha \tilde{p}_k = \partial_x^\alpha p_k$ for all $h = |\alpha| + i + 2 - k$ with $i < h$: If $k < 2$ then $\tilde{p}_k = p_k$ by definition of $\tilde{p}_k$. If, on the other hand, $k = 2$ and $i < h$ then $h = |\alpha| + i + 2 - k = |\alpha| + i$ implies $|\alpha| > 0$ and thus $\partial_\xi^\alpha \tilde{p}_2 = \partial_\xi^\alpha (p_2 - \lambda) = \partial_\xi^\alpha p_2$.

Solving those equations recursively for r_h gives the following definition.

Lemma 3.10. The approximate resolvents $R_N(\lambda)$ for $P - \lambda = \Delta_a^{\mathrm{D}} + Q - \lambda$ are given by the following symbols

$$r_0 \coloneqq 1/\tilde{p}_2 = 1/(\|\xi\|^2 - \lambda) \qquad \text{and}$$
$$r_h \coloneqq -r_0 \sum_{\substack{h=|\alpha|+i+2-k \\ i<h}} \partial_\xi^\alpha p_k \cdot D_x^\alpha r_i/\alpha!\,.$$

Since there are only three nonzero symbols p_0, p_1 and p_2, the latter is equal to

$$\begin{aligned} r_h &= -r_0\Big(\sum_{h=0+i+2-0} p_0 \cdot r_i + \sum_{h=|\alpha|+i+2-1} \partial_\xi^\alpha(-\mathrm{i}\tilde{F}(\xi,x)) \cdot D_x^\alpha r_i/\alpha! \\ &\qquad + \sum_{\substack{h=|\alpha|+i+2-2 \\ i<h}} \partial_\xi^\alpha p_2 \cdot D_x^\alpha r_i/\alpha!\Big) \\ &= -r_0\Big(p_0 r_{h-2} - \mathrm{i}\tilde{F}(\xi,x) r_{h-1} - \mathrm{i}\tilde{F}(e_i,x) D_x^{e_i} r_{h-2} + \partial_\xi^{e_i}\|\xi\|^2 D_x^{e_i} r_{h-1} \\ &\qquad + \partial_\xi^{2e_i}\|\xi\|^2 D_x^{2e_i} r_{h-2}/2\Big) \\ &= -r_0\Big(p_0 r_{h-2} - \mathrm{i}\tilde{F}(\xi,x) r_{h-1} - \tilde{F}(e_i,x)\partial_{x_i} r_{h-2} - 2\mathrm{i}\xi_i \partial_{x_i} r_{h-1} - \partial_{x_i}^2 r_{h-2}\Big) \end{aligned}$$

with $r_h = 0$ for $h < 0$.

Example 3.11. The first two symbols of the sequence of symbols r_h are

$$r_1 = -p_1 r_0^2 = \mathrm{i}\tilde{F}(\xi,x) r_0^2 = \frac{\mathrm{i}\tilde{F}(\xi,x)}{(\|\xi\|^2-\lambda)^2} \qquad \text{and}$$

$$r_2 = -p_0 r_0^2 - p_1^2 r_0^3 = -\Big(\frac{1}{4}\tilde{F}_2(x,x) + Q(x)\Big) r_0^2 - \tilde{F}(\xi,x)^2 r_0^3 .$$

Definition 3.12. As in the proof of [Gil95, Lemma 1.8.1] define

$$e_h(x,\xi,P) \coloneqq (2\pi\mathrm{i})^{-1} \int_\gamma \mathrm{e}^{-\lambda} r_h(x,\xi,\lambda,P)\,\mathrm{d}\lambda$$

$$e_h(x,P) \coloneqq \frac{\operatorname{Vol} M}{(2\pi)^n} \int_{\mathbb{R}^n} e_h(x,\xi,P)\,\mathrm{d}\xi$$

such that by [Gil95, Lemma 1.8.2]

$$K(t,x,x,P) \sim \sum_h e_h(x,P) t^{(h-n)/2} .$$

Here, the curve γ is the boundary of $\mathcal{R}$ as shown in Figure 3.1. The factor $\operatorname{Vol} M$ of the normalization constant $\operatorname{Vol} M/(2\pi)^n$ originates from our choice of scalar product on $\mathrm{L}^2(\omega)$. The factor $(2\pi)^{-n}$ cancels corresponding factors appearing in Fourier transforms. In Gilkey's notation a factor $(2\pi)^{-n/2}$ is "absorbed" in both $\mathrm{d}x$ and $\mathrm{d}\xi$, see [Gil95, page 3].

We proceed to calculate those $e_h(x,P)$.

3.2.1 Integration of λ

The λ-dependency in r_h occurs only in the ${r_0}^k$-terms. For calculating $e_h(x,\xi,P)$, it is therefore sufficient to evaluate

$$\frac{1}{2\pi\mathrm{i}}\int_\gamma \mathrm{e}^{-\lambda}{r_0}^k\,\mathrm{d}\lambda = \frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{\mathrm{e}^{-\lambda}}{(\|\xi\|^2-\lambda)^k}\,\mathrm{d}\lambda = \frac{-(-1)^k}{2\pi\mathrm{i}}\int_{-\gamma}\frac{\mathrm{e}^{-\lambda}}{(\lambda-\|\xi\|^2)^k}\,\mathrm{d}\lambda\,.$$

For $T > \|\xi\|^2$ denote by γ_T the curve that is identical to γ in $\{z\in\mathbb{C} \mid \operatorname{Re} z \le T\}$ and that is closed by a straight line on $\{\operatorname{Re} z = T\}$.

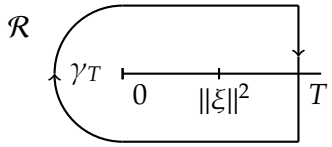


Figure 3.2: The closed approximation γ_T to γ, confer Figure 3.1.

We can approximate the integral over the curve $-\gamma$ above by an integral over the curve $-\gamma_T$ and by the exponential decay of the integrand $\mathrm{e}^{-\lambda}/(\lambda-\|\xi\|^2)^k$ the error is smaller than any $\varepsilon > 0$ for T sufficiently large. Since the integrand is holomorphic in $\lambda\in\mathbb{C}\backslash\{\|\xi\|^2\}$ we can use Cauchy's integral theorem to replace the closed curved $-\gamma_T$ by a counter-clockwise oriented circle δ around $\|\xi\|^2$. Indeed, it follows that

$$\int_{-\gamma}\frac{\mathrm{e}^{-\lambda}}{(\lambda-\|\xi\|^2)^k}\,\mathrm{d}\lambda = \int_\delta \frac{\mathrm{e}^{-\lambda}}{(\lambda-\|\xi\|^2)^k}\,\mathrm{d}\lambda\,.$$

Cauchy's integral formula states that for holomorphic $f\colon U\to\mathbb{C}$, $k\in\mathbb{N}$ and δ a counter-clockwise oriented circle around $z_0 := \|\xi\|^2 \in \mathbb{C}$ we have

$$f^{(k-1)}(z_0) = \frac{(k-1)!}{2\pi\mathrm{i}}\int_\delta \frac{f(z)}{(z-z_0)^k}\,\mathrm{d}z\,.$$

Altogether, we obtain

$$\frac{1}{2\pi\mathrm{i}}\int_\gamma \mathrm{e}^{-\lambda}{r_0}^k\,\mathrm{d}\lambda = (-1)^{k-1}\frac{(-1)^{k-1}}{(k-1)!}\mathrm{e}^{-\|\xi\|^2} = \frac{1}{(k-1)!}\mathrm{e}^{-\|\xi\|^2}\,.$$

Example 3.13. Applying the λ-integration to r_0, r_1 and r_2 yields the following:

$$\begin{aligned}
e_0(x,\xi,P) &= \frac{1}{2\pi\mathrm{i}}\int_\gamma \mathrm{e}^{-\lambda}r_0(x,\xi,\lambda,P)\,\mathrm{d}\lambda = \mathrm{e}^{-\|\xi\|^2}\,,\\
e_1(x,\xi,P) &= \mathrm{i}\tilde{F}(\xi,x)\mathrm{e}^{-\|\xi\|^2} \qquad \text{and}\\
e_2(x,\xi,P) &= -\Big(\frac{1}{4}\tilde{F}_2(x,x)+Q(x)\Big)\mathrm{e}^{-\|\xi\|^2} - \frac{1}{2}\tilde{F}(\xi,x)^2\mathrm{e}^{-\|\xi\|^2}\,.
\end{aligned}$$

3.2.2 Integration of ξ

After the λ-integration each $e_h(x,\xi,P)$ is a sum of terms of the form $A(\xi,\dots,\xi)\cdot e^{-\|\xi\|^2}$, where $A\colon \mathbb{R}^n\times\cdots\times\mathbb{R}^n\to\mathbb{C}$ is a k-multilinear map for some k. Hence, the next step in the calculation of the heat invariants is to evaluate integrals of the form

$$\int_{\mathbb{R}^n} A(\xi,\dots,\xi)\cdot e^{-\|\xi\|^2}\,d\xi\,.$$

If k is odd then the integrand is odd and thus the integral vanishes. We can assume that $k=2s$ for some $s\in\mathbb{N}_0$. With the *double factorial*

$$k!! := k\cdot(k-2)!! \qquad \text{with } (-1)!!:=1 \text{ and } 0!!:=1$$

we can express the integral in dimension one as follows:

Lemma 3.14. $$\int_{\mathbb{R}}\xi^{2s}e^{-\xi^2}\,d\xi=\frac{\sqrt{\pi}}{2^s}(2s-1)!!$$

Proof.

$$\begin{aligned}\int_{\mathbb{R}}\xi^{2s}e^{-\xi^2}\,d\xi &= (-1)^s\int_{\mathbb{R}}\partial^s_{a=1}e^{-\xi^2 a}\,d\xi=(-1)^s\partial^s_{a=1}\int_{\mathbb{R}}e^{-\xi^2 a}\,d\xi\\ &=(-1)^s\partial^s_{a=1}\sqrt{\frac{\pi}{a}}=(-1)^s\sqrt{\pi}\cdot\partial^s_{a=1}a^{-1/2}=(-1)^s\sqrt{\pi}\cdot\Big(-\frac12\Big)\cdots\Big(-\frac{2s-1}{2}\Big)\\ &=\sqrt{\pi}\frac{1}{2^s}(2s-1)!!\qquad\square\end{aligned}$$

Example 3.15. The preceding lemma gives the following for a bilinear map $A\colon\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{C}$:

$$\begin{aligned}\int_{\mathbb{R}^n}A(\xi,\xi)\cdot e^{-\|\xi\|^2}\,d\xi &= A(e_i,e_j)\int_{\mathbb{R}^n}\xi^i\xi^j\cdot e^{-\|\xi\|^2}\,d\xi\\ &=A(e_i,e_j)\delta^{ij}\frac{\sqrt{\pi}^n}{2}(2-1)!!=\operatorname{Tr}A\frac{\sqrt{\pi}^n}{2}\,.\end{aligned}$$

For the integral in the general setting we need a concept of a trace for $2s$-multilinear maps.

Definition 3.16 (Multitrace).
For $k=2s$ let $P(k)$ denote the set of all partitions of $\{1,\dots,k\}$ into pairs, i. e. $p=\{p_1,\dots,p_s\}\in P(k)$ if $\#p_i=2$ and $\bigcup p_i=\{1,\dots,k\}$. For $p\in P(k)$ and some multiindex $i\in M^k(n):=\{1,\dots,n\}^k$ let

$$\delta_p(i):=\begin{cases}1 & \text{if } i_{p_{j,1}}=i_{p_{j,2}} \text{ for all } j=1,\dots,s\\ 0 & \text{otherwise.}\end{cases}$$

In other words, $\delta_p(i)$ is one if and only if the entries in the multiindex i agree on the pairs in p. If $i \in \{1, \dots, n\}$ then e_i shall denote the i-th standard basis vector of $\mathbb{R}^n$. For $i \in M^k(n)$ abbreviate $e_i \coloneqq (e_{i_1}, \dots, e_{i_k}) \in (\mathbb{R}^n)^k$.

Define the multitrace of a $2s$-multilinear map A as

$$\operatorname{Tr} A \coloneqq \sum_{p \in P(2s)} A(e_i)\delta_p(i) \qquad \text{(with Einstein convention).}$$

Here the Einstein convention is understood as summing over all multiindices $i \in M^k(n)$.

Example 3.17. If $k = 2$ then $P(2) = \{\{\{1,2\}\}\}$ and

$$\operatorname{Tr} A = \sum_{p \in P(2)} A(e_{i_1}, e_{i_2})\delta_p(i_1, i_2) = A(e_{i_1}, e_{i_1}) = A(e_i, e_i)\,.$$

Thus, for $k = 2$ the multitrace is just the usual trace with respect to the standard inner product.

Example 3.18. If $k = 4 = 2 \cdot 2$ then

$$\begin{aligned} P(4) = \{&\{\{1,2\},\{3,4\}\},\\ &\{\{1,3\},\{2,4\}\},\\ &\{\{1,4\},\{2,3\}\}\} \end{aligned}$$

and the multitrace of a 4-multilinear map A is given by

$$\operatorname{Tr} A = A(e_i, e_i, e_j, e_j) + A(e_i, e_j, e_i, e_j) + A(e_i, e_j, e_j, e_i)\,.$$

Remark 3.19. Note that $\operatorname{Tr} A$ is independent of the choice of orthonormal basis $\{e_i\}_{i \in \{1,\dots,n\}}$, because each summand of the trace consists of evaluating the conventional trace several times and because the trace of bilinear maps is independent of the choice of orthonormal basis.

Also, the curvature trace F_2, see Definition 3.7, differs from the multitrace of the 4-multilinear map $F \cdot F$. By Example 3.18

$$\operatorname{Tr}(F \cdot F) = F(e_i, e_i)F(e_j, e_j) + F(e_i, e_j)F(e_i, e_j) + F(e_i, e_j)F(e_j, e_i) = 0$$

for antisymmetric F. However, we can easily choose antisymmetric F such that $F_2 = F(e_i, e_j) \cdot F(e_j, e_i) \neq 0$.

Theorem 3.20. For a k-multilinear map $A\colon \mathbb{R}^n \times \cdots \times \mathbb{R}^n \to \mathbb{C}$ with $k = 2s$ for some $s \in \mathbb{N}_0$ we have

$$\int_{\mathbb{R}^n} A(\xi, \dots, \xi) \cdot \mathrm{e}^{-\|\xi\|^2}\, \mathrm{d}\xi = \frac{\pi^{n/2}}{2^s} \operatorname{Tr} A\,.$$

If k is odd then the integral vanishes.

Proof. First note that both sides of the equation are linear in A. It therefore suffices to show this claim for elementary multilinear maps of the form

$$A_i(e_j) \coloneqq \delta_i(j) \qquad \text{for multiindices } i, j \in M^k(n)\,.$$

For those maps we have

$$\operatorname{Tr} A_i = \sum_{p \in P(k)} A_i(e_j)\delta_p(j) = \sum_{p \in P(k)} \delta_p(i)\,.$$

Thus, $\operatorname{Tr} A_i$ gives the number of partitions of $\{1,\dots,k\}$ into pairs that are compatible with i. Now, let $\hat{i} \in \mathbb{N}^n$ be defined by

$$\hat{i}_h \coloneqq \#\{t \mid i_t = h\}\,,$$

i. e. $\hat{i}_h$ is the number of indices in i with value h. If $\hat{i}$ is not even, that is, if not all of its entries are even, then $\operatorname{Tr} A_i = 0$. If it is even then

$$\operatorname{Tr} A_i = (\hat{i}-1)!! \coloneqq \prod_{h=1}^{n} (\hat{i}_h - 1)!!\,,$$

since there are $(t-1)!!$ pairings for every set with t elements, t even.

On the other hand, if $\hat{i} = 2\alpha$ is even, then

$$\begin{aligned}\int_{\mathbb{R}^n} A_i(\xi,\dots,\xi)\cdot \mathrm{e}^{-\|\xi\|^2}\,\mathrm{d}\xi &= \int_{\mathbb{R}^n} \xi^{i_1}\cdots\xi^{i_k}\cdot \mathrm{e}^{-\|\xi\|^2}\,\mathrm{d}\xi \\ &= \int_{\mathbb{R}^n} \xi^{\hat{i}}\mathrm{e}^{-\|\xi\|^2}\,\mathrm{d}\xi = \prod_{h=1}^{n}\int_{\mathbb{R}} \xi^{\hat{i}_h}\mathrm{e}^{-(\xi^h)^2}\,\mathrm{d}\xi = \prod_{h=1}^{n}\frac{\sqrt{\pi}}{2^{\alpha_h}}(\hat{i}_h-1)!!\end{aligned}$$

by Lemma 3.14 and the integral vanishes if $\hat{i}$ is not even. It follows that

$$\int_{\mathbb{R}^n} A_i(\xi,\dots,\xi)\cdot \mathrm{e}^{-\|\xi\|^2}\,\mathrm{d}\xi = \frac{\pi^{n/2}}{2^s}\operatorname{Tr} A_i\,.$$

□

Corollary 3.21 ([Gil95, Lemma 1.8.2 (d)]).
If h is odd then

$$e_h(x,P) = 0\,.$$

Proof. The symbols r_h of the $R_N(\lambda)$ are sums of terms of the form $A(\xi,\dots,\xi){r_0}^j$ and the λ-integration converts $A(\xi,\dots,\xi){r_0}^j$ into $A(\xi,\dots,\xi)\mathrm{e}^{-\|\xi\|^2}/(j-1)!$. By Theorem 3.20 ξ-integrations vanish if the involved multilinear form A has an odd number of arguments. It, therefore, suffices to show that all A within r_h have an odd number of ξ-arguments if h is odd.

This claim is true for r_0 and $r_1 = \mathrm{i}\tilde{F}(\xi, x)r_0^2$. For r_h with $h > 1$ we have

$$r_h = -r_0(p_0 r_{h-2} - \mathrm{i}\tilde{F}(\xi, x)r_{h-1} - \tilde{F}(e_i, x)\partial_{x_i} r_{h-2} - 2\mathrm{i}\xi_i \partial_{x_i} r_{h-1} - \partial_{x_i}^2 r_{h-2})$$

by Definition 3.10 where $p_0(x, \xi)$ is constant in ξ. The claim follows by induction. □

Example 3.22. Continuing with the ξ-integration of the $e_i(x, \xi, P)$ of Example 3.13 we have

$$\begin{aligned} e_0(x, P) &= \frac{\operatorname{Vol} M}{(2\pi)^n}\pi^{n/2} = \operatorname{Vol} M(4\pi)^{-n/2} \\ e_1(x, P) &= 0 \\ e_2(x, P) &= \frac{\operatorname{Vol} M}{(2\pi)^n}\Big(-(\frac{1}{4}\tilde{F}_2(x, x) + Q(x))\pi^{n/2} - \frac{1}{2}\tilde{F}(e_i, x)^2\frac{\pi^{n/2}}{2}\Big) \\ &= -Q(x)\operatorname{Vol} M(4\pi)^{-n/2}, \end{aligned}$$

because $\tilde{F}(e_i, x)^2 = -\tilde{F}(x, e_i)\tilde{F}(e_i, x) = -\tilde{F}_2(x, x)$ (with the Einstein convention, of course). When comparing those results with the ones obtained using the MATHEMATICA notebook of Appendix C note that the factors $\operatorname{Vol} M(4\pi)^{-n/2}$ have been omitted on purpose in the notebook.

3.3 Results

Assume that a nondegenerate line bundle ω over a flat torus $M = \mathbb{R}^n/\mathcal{L}$, a translation-invariant connection $a \in \mathbb{R}^{n\prime}$ and some potential Q on M are given. Because for $t \to 0$

$$\sum_{k\in\mathbb{N}} \mathrm{e}^{-t\lambda_k} = \frac{1}{\operatorname{Vol} M}\int_M \operatorname{Tr}_{\omega_x} K(t, x, x, P)\,\mathrm{d}x \sim \sum_{k\in\mathbb{N}} \frac{1}{\operatorname{Vol} M}\int_M e_k(x, P)\,\mathrm{d}x\, t^{(k-n)/2}$$

it follows that the

$$a_k(P) \coloneqq \frac{1}{\operatorname{Vol} M}\int_M e_k(x, P)\,\mathrm{d}x$$

are spectral invariants of P. The trace can be omitted since ω is a line bundle. The first three heat invariants are easy to calculate:

Example 3.23.

$$\begin{aligned} a_0(P) &= \frac{1}{\operatorname{Vol} M}\int_M \operatorname{Vol} M(4\pi)^{-n/2}\,\mathrm{d}x = (4\pi)^{-n/2}\cdot\operatorname{Vol} M \\ a_1(P) &= 0 \qquad \text{and} \\ a_2(P) &= -(4\pi)^{-n/2}\cdot\frac{1}{\operatorname{Vol} M}\int_M Q(x)\operatorname{Vol} M\,\mathrm{d}x = -(4\pi)^{-n/2}Q_0\operatorname{Vol} M. \end{aligned}$$

In fact, Corollary 3.21 implies that all odd heat invariants are zero. Q_0 is the Fourier coefficient with respect to E_0, see Definition 2.2.

Remark 3.24. As in [Gil95, Theorem 4.2.1] it follows from this asymptotic expansion and the fact that $a_0(P) \neq 0$ that the dimension n and hence the volume $\operatorname{Vol} M$ of the torus M are spectral invariants. Furthermore, the average Q_0 of the potential Q is also a spectral invariant.

Since the dimension n and $\operatorname{Vol} M$ are spectral invariants it follows that if $a_k(P)$ is a spectral invariant then so is $\frac{(4\pi)^{n/2}}{\operatorname{Vol} M} \cdot a_k(P)$. Therefore:

Definition 3.25. Denote the (*unintegrated*) *heat invariants* by

$$\mathsf{hi}_k(x,P) := \frac{(4\pi)^{n/2}}{\operatorname{Vol} M} \cdot e_k(x,P) \qquad \text{and}$$
$$\mathsf{hi}_k(P) := \frac{1}{\operatorname{Vol} M} \int_M \mathsf{hi}_k(x,P)\,\mathrm{d}x\,.$$

While we cannot perform the x-integration outright without a more specific choice of potential Q, we can use integration by parts to simplify the heat invariants.

Lemma 3.26 (Integration by Parts).
If $f, g\colon \mathbb{R}^n \to \mathbb{C}$ are two $\mathcal{L}$-periodic smooth function and $\mathcal{F}$ a unit cell of $\mathcal{L}$, then

$$\int_{\mathcal{F}} \partial_i f \cdot g \,\mathrm{d}x = -\int_{\mathcal{F}} f \cdot \partial_i g \,\mathrm{d}x\,.$$

See Appendix C for more details.

Since we are only interested in the unintegrated heat invariants $\mathsf{hi}_k(x,P)$ up to integration with respect to x we use the following abbreviation.

Definition 3.27. Given two smooth $\mathcal{L}$-periodic functions $f, g\colon \mathbb{R}^n \to \mathbb{C}$ write

$$f \approx g \qquad \text{if} \qquad \int_M f(x)\,dx = \int_M g(x)\,\mathrm{d}x\,.$$

For example, we write $(\partial_i f)g \approx -f(\partial_i g)$. Also, if $\mathsf{hi}_k(x,P) \approx H(x)$ then $\mathsf{hi}_k(P) = \int_M \mathsf{hi}_k(x,P)\,\mathrm{d}x = \int_M H(x)\,\mathrm{d}x$.

It is possible to compute all necessary derivations and integrations needed to obtain the heat invariants manually. This would be prohibitively labor intensive for higher invariants, however. Those computations, the mentioned integration by parts and some other simplifications are implemented in a MATHEMATICA notebook given in Appendix C. This notebook returns the following (unintegrated) heat invariants.

Recall that we have used "function overloading" Definition 3.7 of the curvature traces: If $\tilde{F}_k$ appears without arguments, it is understood that

$$\tilde{F}_k = \tilde{F}_k(e_i, e_i)\,.$$

Theorem 3.28 (Heat Invariants).
Given an even-dimensional flat torus M, a nondegenerate Hermitian line bundle ω over M, a translation-invariant connection $a \in \mathbb{R}^{n'}$ on this bundle and a smooth potential Q on M then the (unintegrated) heat invariants of the Schrödinger operator $P \coloneqq \Delta_a^{\mathrm{D}} + Q$ are given by the following formulae:

$$\begin{aligned}
\mathsf{hi}_0(x,P) &= 1\\
\mathsf{hi}_2(x,P) &= -Q(x)\\
\mathsf{hi}_4(x,P) &\approx -\frac{\tilde{F}_2}{12} + \frac{1}{2}Q(x)^2\\
\mathsf{hi}_6(x,P) &\approx \frac{\tilde{F}_2}{12}Q(x) + \frac{Q(x)\Delta Q(x)}{12} - \frac{Q(x)^3}{6}\\
\mathsf{hi}_8(x,P) &\approx \frac{(\tilde{F}_2)^2}{288} + \frac{\tilde{F}_4}{360} + \frac{Q(x)\Delta^2 Q(x)}{120} - \frac{\tilde{F}_2}{24}Q(x)^2\\
&\quad - \frac{Q(x)^2\Delta Q(x)}{24} + \frac{1}{24}Q(x)^4\\
\mathsf{hi}_{10}(x,P) &\approx \Big(-\frac{(\tilde{F}_2)^2}{288} - \frac{\tilde{F}_4}{360}\Big)Q(x) - \frac{1}{180}Q(x)\tilde{F}_2(e_i,e_j)\partial_i\partial_j Q(x)\\
&\quad - \frac{\tilde{F}_2}{144}Q(x)\Delta Q(x) + \frac{1}{1680}Q(x)\Delta^3 Q(x)\\
&\quad + \frac{1}{72}\Big(\tilde{F}_2\,Q(x)^3 - \frac{1}{5}Q(x)(\Delta Q(x))^2 - \frac{1}{5}Q(x)^2\Delta^2 Q(x)\Big)\\
&\quad + \frac{1}{72}Q(x)^3\Delta Q(x) - \frac{Q(x)^5}{120}
\end{aligned}$$

The heat invariants $\mathsf{hi}_{12}(x,P)$ and $\mathsf{hi}_{14}(x,P)$ can be found in the MATHEMATICA notebook of Appendix C.

The Einstein convention is used in hi_{10}; the variables i and j are summed over $\{1,\dots,n\}$. The Laplacian used to express the heat invariants is defined as $\Delta \coloneqq \partial_i^2$. Integration over M gives the spectral invariants

$$\mathsf{hi}_k(P) = \frac{1}{\operatorname{Vol} M}\int_M \mathsf{hi}_k(x,P)\,\mathrm{d}x\,.$$

Remark 3.29. Note that the heat invariants 0 to 6 given in Theorem 3.28 agree with those given in [Gil95, Theorem 4.1.6]. To see this observe that (in Gilkey's notation)

$$E = -Q\,.$$

Also, Gilkey's R, ρ and τ are the curvature, Ricci tensor and the scalar curvature. All three vanish on flat tori. Further, partial integration gives

$$E_{;kk} = -\partial_k^2 Q \approx \partial_k Q \cdot \partial_k 1 = 0$$

and for the curvature terms of $\nabla^{A^{\mathrm{D}}+a}$ we have

$$\Omega_{ij}\Omega_{ij} = \tilde{F}(e_i, e_j)\tilde{F}(e_i, e_j) = -\tilde{F}(e_i, e_j)\tilde{F}(e_j, e_i) = -\tilde{F}_2\,.$$

Overall, we have, for example, in Gilkey's notation:

$$\begin{aligned} e_4(x, D) = (4\pi)^{-n/2}\frac{1}{360}\Big(&60E_{;kk} + 60\tau E + 180E^2 \\ &+ (12\tau_{;kk} + 5\tau^2 - 2|\rho|^2 + 2|R|^2)I_V + 30\Omega_{ij}\Omega_{ij}\Big) \\ &= (4\pi)^{-n/2}\Big(\frac{1}{2}Q(x)^2 - \frac{1}{12}\tilde{F}_2\Big) = (4\pi)^{-n/2}\mathsf{hi}_4(x, P)\,. \end{aligned}$$

Similarly, we recognize Gilkey's $e_6(x, D)$ as our $(4\pi)^{-n/2}\mathsf{hi}_6(x, P)$ by using $\Omega_{ij;k} = 0$, $Q_iQ_i \approx -Q\Delta Q$, $\Delta^2 Q \approx 0$ and the fact that for odd k we have $\tilde{F}_k = 0$ by Lemma 3.9.

It should be noted again that the translation-invariant connection $a \in \mathbb{R}^{n'}$ does not appear in the heat invariants and those invariants can therefore not provide any spectral information on those connections. For information on the connections we need the wave invariants, whose computation is the main goal of this thesis.

Prior to this we consider a particularly simple scenario: constant potentials.

3.4 Constant Potentials

The case of constant potentials is very simple and the isospectrality relations can be described completely.

Theorem 3.30. Fix a nondegenerate line bundle ω over an even-dimensional torus M such that the translation-invariant connections have the curvature form $-2\pi\mathrm{i}F$. Assume that $Q, P \in C^\infty(M)$ are two smooth potentials that are isospectral with respect to the Laplacian Δ_a^{D} of some translation-invariant connection $a \in \mathbb{R}^{n'}$. If Q is constant then P is constant and

$$Q = P\,.$$

Proof. The second heat invariant is

$$\mathsf{hi}_2(P) = \frac{1}{\operatorname{Vol} M}\int_M -Q(x)\,\mathrm{d}x = -Q_0$$

and the fourth is

$$\mathsf{hi}_4(P) = \frac{1}{\operatorname{Vol} M}\int_M -\frac{\tilde{F}_2}{12} + \frac{1}{2}Q(x)^2\,\mathrm{d}x = -\frac{\tilde{F}_2}{12} + \frac{1}{2}\|Q\|^2\,.$$

Because $\tilde{F}_2$ is a constant, $\|Q\|^2$ is a spectral invariant. It follows that $Q_0 = P_0$ and

$$\|P\|^2 = \|Q\|^2 = Q_0^2 = P_0^2\,.$$

This in turn implies, by $\|P\|^2 = \|P_0\|^2 + \|P - P_0\|^2$, that P must be constant. Hence, $P = Q$. □

Remark 3.31. On the other hand, we have by Corollary 2.15 that for a constant potential $Q = Q_0$ all translation-invariant connections $a \in \mathbb{R}^{n\prime}$ are isospectral.

The preceding remark together with Theorem 3.30 completely describes the isospectrality relations in the case of constant potentials.

Chapter 4

Wave Invariants

Similarly to the heat equation and the heat invariants we will study the wave equation of the operator $P \coloneqq \Delta_a^{\mathrm{D}} + Q$ to compute wave invariants and obtain information provided by the spectrum of P. The wave trace will be a distribution with more singularities complicating the analysis but also providing more information. We will not concentrate on distribution theory but instead pick up on the idea presented in the appendix of [GGKW08]. There, the first wave invariant was calculated and some information about the second wave invariant was given.

We will formulate this computation more explicitly, which allows us to use MATHEMATICA to compute the first five wave invariants, see Appendix D. We can also draw more general conclusions about wave invariants of any order.

In this chapter we will outline the construction of the wave trace in general and on the line bundle ω. An explicit algorithm, a recipe, for the calculation of the spectrally invariant coefficients of the wave trace expansion is given in Section 4.4. With this recipe at hand we will start with computing the first two wave invariants manually. This will not only familiarize the reader with the computation of wave invariants, but we will also introduce abbreviations, so-called *notations*, that shorten the computation and that are used in the MATHEMATICA notebook of Appendix D available in digital form in [Ber18].

4.1 The Wave Trace

We will begin with the definition of the wave trace and its spectral implications. An introduction to distribution theory can be found in [FJ98] or more specifically for distributions on vector bundles and wave operators in [Bär10]. For a detailed explanation of traces of elliptic differential operators see [AB67].

Definition 4.1. For for a smooth time-dependent section $u \in \mathcal{E}_t(\omega)$, see Definition 3.2 the equation

$$\begin{aligned} &\big(\partial_t^2 + P\big)u(t,x) = 0 \qquad \text{with the initial conditions} \\ &u(0,x) = u_0(x) \quad \text{and} \quad \partial_t u(0,x) = 0 \qquad \text{for all } x \in M \text{ and } t \in \mathbb{R} \end{aligned}$$

with $u_0 \in \mathcal{E}(\omega)$ is called *wave equation* of $P = \Delta_a^{\mathrm{D}} + Q$.

We can use the discrete spectral resolution $\{\phi_k, \lambda_k\}$ of P given in [Gil95, Lemma 1.6.3] and the *functional calculus* to define a one-parameter family of bounded operators

$$K_t \coloneqq \cos(t\sqrt{P}) \colon \mathcal{E}(\omega) \to \mathcal{E}(\omega)$$

that is smooth with respect to t and such that $K_t u_0$ solves the wave equation for any initial condition $u_0 \in \mathcal{E}(\omega)$. Note that this *wave operator* is well-defined even though $P = \Delta_a^{\mathrm{D}} + Q$ is, in general, not positive semi-definite and may have negative eigenvalues. This *wave operator* K_t has a distributional kernel in $\mathcal{D}'(\omega \boxtimes \omega^*)$ given by

$$\begin{aligned} K_t(x,y) &= \sum_{i=1}^{\infty} \cos(t\sqrt{\lambda_i})\phi_i(x) \boxtimes \phi_i^*(y)\,, \qquad \text{which means} \\ K_t(\phi \boxtimes \psi) &= \frac{1}{\operatorname{Vol} M^2} \sum_{i=1}^{\infty} \cos(t\sqrt{\lambda_i}) \int_{M\times M} \langle \phi_i(x), \phi(x)\rangle \cdot \langle \phi_i(y), \psi(y)\rangle \,\mathrm{d}x\mathrm{d}y\,. \end{aligned}$$

The normalization factor $1/\operatorname{Vol} M^2$ follows from the fact that we have defined our scalar product on $\mathrm{L}^2(\omega)$ with a normalization factor $1/\operatorname{Vol} M$, see Definition 3.1. It follows that the trace of the wave operator is given by

$$\operatorname{trace} K_t = \sum_{i=1}^{\infty} \cos(t\sqrt{\lambda_i})\phi_i^*(\phi_i) = \sum_{i=1}^{\infty} \cos(t\sqrt{\lambda_i})\,.$$

In particular, this so-called *wave trace* is a spectral invariant of $\Delta_a^{\mathrm{D}} + Q$.

Lemma 4.2. If $\operatorname{Spec}_a(Q,\omega) = \{\lambda_1, \lambda_2, \dots\}$ is the spectrum of the operator $\Delta_a^{\mathrm{D}} + Q$ then $\sum_{i=1}^{\infty} \cos(\,\cdot\,\sqrt{\lambda_i})$ is a well-defined distribution on $\mathbb{R}$.

Proof. By [Gil95, Lemmata 1.6.3 and 1.6.4] we have for the spectrum $\operatorname{Spec}_a(Q,\omega)$ that there exists an $\epsilon > 0$ and a constant $C > 0$ such that $\lambda_i \geq Ci^{\epsilon}$ for all i greater than or equal to some i_0. Choose an even $k \in \mathbb{N}$ such that $\epsilon \cdot k/2 > 1$.

The definition of a distribution is given in [FJ98, Section 1.3]. Fix a compact set $K \subset \mathbb{R}$. For all smooth, compactly supported test functions $\phi \in \mathcal{D}(\mathbb{R})$ with

supp $\phi \subset K$ we have with k partial integrations that

$$\begin{aligned}\Big|\langle\sum_{i=1}^{\infty}\cos(\,.\cdot\sqrt{\lambda_i}),\phi\rangle\Big| &\le \sum_{i=1}^{\infty}\Big|\int_{\mathbb{R}}\cos(t\sqrt{\lambda_i})\cdot\phi(t)\,\mathrm{d}t\Big| \\ &\le C_K\cdot\sup_{t\in K}|\phi(t)| + \sum_{i=i_0}^{\infty}\Big|\int_{\mathbb{R}}\frac{1}{\sqrt{\lambda_i}^k}\cos(t\sqrt{\lambda_i})\cdot\phi^{(k)}(t)\,\mathrm{d}t\Big| \\ &\le C_K\cdot\sup_{t\in K}|\phi(t)| + \sum_{i=i_0}^{\infty}\frac{1}{\lambda_i^{k/2}}\int_{\mathbb{R}}|\phi^{(k)}(t)|\,\mathrm{d}t\end{aligned}$$

with some constant $C_K > 0$. Note that no sine remains in the partial integrations, because we have chosen k to be even. The generalized harmonic series converges and thus

$$\Big|\langle\sum_{i=1}^{\infty}\cos(\,.\cdot\sqrt{\lambda_i}),\phi\rangle\Big| \le C_K\cdot\sup_{t\in K}|\phi(t)| + C'\cdot\sup_{t\in K}|\phi^{(k)}|\,.$$

It follows that $\sum_{i=1}^{\infty}\cos(\,.\cdot\sqrt{\lambda_i})$ is both well-defined and continuous as linear map $\mathcal{D}(\mathbb{R})\to\mathbb{C}$. □

4.2 The Wave Equation on $\mathbb{R}^n$

We will now compute an asymptotic expansion of the wave trace in its singularities. We start by computing an approximate wave kernel for the wave equation on $\mathbb{R}^n$. This approximation will use the concepts of *oscillatory integrals* and their *symbols*. More details and proofs of the corresponding theorems can be found in [Dui96] and [GS94].

Let $X \subset \mathbb{R}^N$ denote an open subset of $\mathbb{R}^N$ and write $\dot{\mathbb{R}}^n := \mathbb{R}^n\backslash\{0\}$.

Definition 4.3. For any $m \in \mathbb{R}$ let $S^m := S^m(X\times\mathbb{R}^n)$ denote the set of symbols of order m, which are the smooth functions $a \in C^\infty(X\times\mathbb{R}^n)$ such that for all multiindices α, β and every compact $K \subset X$ there is a constant C with

$$|\partial_x^\alpha\partial_\theta{}^\beta a(x,\theta)| \le C(1+|\theta|)^{m-|\beta|} \qquad \text{for all } (x,\theta)\in K\times\mathbb{R}^n.$$

Minimal constants C define seminorms on S^m that define a locally convex topology on S^m.

Abbreviate, $S^{-\infty} := \bigcap_{m\in\mathbb{R}} S^m$ and $S^\infty := \bigcup_{m\in\mathbb{R}} S^m$. We call the symbols in $S^{-\infty}$ *smoothing*.

We denote symbols by a or a_i to stay in the notation of [GGKW08]. They should not to be confused with a translation-invariant connection given by some $a \in \mathbb{R}^{n\prime}$ as in Notation 1.24.

Example 4.4. A function $a \in C^\infty(X \times \dot{\mathbb{R}}^n)$ is called *positively homogeneous* of degree $m \in \mathbb{R}$, if for all $c \in \mathbb{R}$ with $c > 0$ and all $(x, \theta) \in X \times \dot{\mathbb{R}}^n$ we have $a(x, c\theta) = c^m a(x, \theta)$.

If $a \in C^\infty(X \times \dot{\mathbb{R}}^n)$ is positively homogeneous of degree $m \in \mathbb{R}$ and if $\chi \in C^\infty(\mathbb{R}^n, [0, 1])$ is a smooth cut-off function equal to 0 in a neighborhood of $0 \in \mathbb{R}^n$ and equal to 1 outside some compact set around $0 \in \mathbb{R}^n$, then $X \times \mathbb{R}^n \ni (x, \theta) \mapsto \chi(\theta) a(x, \theta) \in \mathbb{C}$ is a symbol of order m.

The following proposition can be found in [Dui96, Proposition 2.1.2] or [Gil95, Lemma 1.2.9].

Proposition 4.5. If we are given a sequence of symbols $a_i \in S^{m_i}$ of decreasing order $m_i \to -\infty$, then there exists a symbol $a \in S^{m_0}$ with

$$a \sim \sum_{i=1}^{\infty} a_i \quad \text{more precisely} \quad a - \sum_{i=1}^{k} a_i \in S^{m_{k+1}} \quad \text{for all } k \in \mathbb{N}.$$

The symbol a is unique up the addition of smoothing symbols and is called *resummation* of the sequence $(a_i)_{i \in \mathbb{N}}$.

Definition 4.6. A function $\phi \in C^\infty(X \times \dot{\mathbb{R}}^n)$ is called a *phase function* if its imaginary part satisfies $\operatorname{im} \phi \geq 0$, $\mathrm{d}\phi \neq 0$ and if ϕ is positively homogeneous of degree 1.

The following Theorem can be found in [GS94, Theorem 1.11] and [Dui96, Theorem 2.2.1].

Theorem 4.7. If ϕ is a phase function and $a \in S^m$ a symbol of sufficiently small order, that is $m + h < -n$, then

$$I(a, \phi) := \int \mathrm{e}^{\mathrm{i}\phi(\,.\,,\theta)} a(\,.\,,\theta)\, \mathrm{d}\theta \in C^h(X) \subset \mathcal{D}'(X)$$

and there is a unique extension

$$I(\,.\,, \phi) \colon S^\infty \to \mathcal{D}'(X)$$

that is continuous on S^m for all $m \in \mathbb{R}$. For $a \in S^\infty$ this extension $I(a, \phi) \in \mathcal{D}'(X)$ is called *oscillatory integral* and can be formally written as

$$I(a, \phi)(x) = \int \mathrm{e}^{\mathrm{i}\phi(x,\theta)} a(x, \theta)\, \mathrm{d}\theta \qquad \text{and}$$

$$\langle I(a, \phi), u \rangle = \iint \mathrm{e}^{\mathrm{i}\phi(x,\theta)} a(x, \theta) u(x)\, \mathrm{d}x \mathrm{d}\theta\,.$$

If $a \in S^{-\infty}$ is a smoothing symbol, then $I(a, \phi)$ is a smooth map.

We now fix a specific domain $X \coloneqq \mathbb{R}^n \times \mathbb{R}^n$ to continue with our computation. If ϕ a phase function on $(\mathbb{R}^n \times \mathbb{R}^n) \times \dot{\mathbb{R}}^n$ and $a \in S^m((\mathbb{R}^n \times \mathbb{R}^n) \times \mathbb{R}^n)$ then $I(a, \phi) \in \mathcal{D}'(\mathbb{R}^n \times \mathbb{R}^n)$ can be considered as the distributional kernel of an operator. This operator shall be formally written as

$$Bu(x) = \iint \mathrm{e}^{\mathrm{i}\phi(x,y,\theta)} a(x, y, \theta) u(y) \, \mathrm{d}y \mathrm{d}\theta \qquad \text{for } u \in \mathcal{D}(\mathbb{R}^n).$$

Definition 4.8. For $X = \mathbb{R}^n \times \mathbb{R}^n$ and $t \in \mathbb{R}$ we define two types of phase functions $\phi^\pm(t, \,.\,) \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n \times \dot{\mathbb{R}}^n)$ by

$$\phi^\pm(t, x, y, \theta) \coloneqq (x - y) \cdot \theta \pm t|\theta| \qquad \text{for all } (x, y, \theta) \in \mathbb{R}^n \times \mathbb{R}^n \times \dot{\mathbb{R}}^n.$$

We abbreviate $\phi^\pm(t, x, \theta) = \phi^\pm(t, x, 0, \theta)$.

Given a translation-invariant connection $\tilde{a}$ on a line bundle ω and a potential Q on the torus $M = \mathbb{R}^n / \mathcal{L}$ we can view the Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$ as a differential operator acting on the $\mathcal{L}$-equivariant complex-valued functions on $\mathbb{R}^n$.

Definition 4.9. We define the *box operator* as

$$\Box \coloneqq \partial_t{}^2 + P = \partial_t{}^2 + \Delta_a^{\mathrm{D}} + Q \,.$$

In the literature the box or d'Alembert operator denotes $\partial_t^2 + \Delta$, but for our purposes it is convenient to include the potential Q. We will also call the d'Alembert operator wave operator and trust that it will be clear from the context whether K_t or $\Box$ is referred to.

The aim of this section is to find an approximation to the wave operator $K_t = \cos(t\sqrt{P})$ on $\mathbb{R}^n$. Following [GGKW08, Appendix A] we consider the ansatz

$$\begin{aligned} K_t^\pm u(x) &= \iint \mathrm{e}^{\mathrm{i}\phi^\pm(t,x,y,\theta)} a^\pm(t, x, \theta) u(y) \, \mathrm{d}y \mathrm{d}\theta \\ &= \int \mathrm{e}^{\mathrm{i}\phi^\pm(t,x,\theta)} a^\pm(t, x, \theta) \hat{u}(\theta) \, \mathrm{d}\theta \end{aligned}$$

with $K_t = (K_t^+ + K_t^-)/2$. Here, $a^\pm(t, \,.\,, \,.\,)$ are suitable symbols on $\mathbb{R}^n \times \mathbb{R}^n$. Because differentiation is a continuous map between spaces of symbols, we have that

$$\Box K_t^\pm u = \int \Box\Big(\mathrm{e}^{\mathrm{i}\phi^\pm(t,\,.\,,\theta)} a^\pm(t, \,.\,, \theta)\Big) \hat{u}(\theta) \, \mathrm{d}\theta$$

and we want, heuristically, that $\Box K_t^\pm u \approx 0$. This can be achieved by constructing the symbols $a^\pm$ as the resummation of a sequence $a_i^\pm$ of symbols of order $-i$ for which $\Box\Big(\mathrm{e}^{\mathrm{i}\phi^\pm} \sum_{i=1}^\infty a_i^\pm\Big)$ is a telescoping series.

Such a resummation will be constructed in the remainder of this section.

Lemma 4.10. With $A = A^{\mathrm{D}} + \tilde{a}$, using Proposition 1.35 and the definition of $\phi^{\pm}$ we easily obtain

$$\Box\Big(\mathrm{e}^{\mathrm{i}\phi^{\pm}} \sum_{i=0}^{N} a_i^{\pm}\Big)(t,x,\theta) = \\ \mathrm{e}^{\mathrm{i}\phi^{\pm}(t,x,\theta)}\Big(\Box - 2\mathrm{i}A_x(\theta) \pm 2\mathrm{i}|\theta|\partial_t - 2\mathrm{i}\,\theta\cdot\operatorname{grad}_x\Big)\sum_{i=0}^{N} a_i^{\pm}(t,x,\theta)\,. \quad (*)$$

There are smooth functions $a_i^{\pm} \in C^{\infty}(\mathbb{R}\times\mathbb{R}^n\times\dot{\mathbb{R}}^n)$ positive-homogeneous of degree $-i$, which solve the following transport equations:

$$2\mathrm{i}\Big(-A_x(\theta) \pm |\theta|\partial_t - \theta\cdot\operatorname{grad}_x\Big)a_i^{\pm}(t,x,\theta) + \Box a_{i-1}^{\pm}(t,x,\theta) = 0 \qquad (**)$$

with the initial conditions

$$a_0^{\pm}(0,x,\theta) = 1 \qquad \text{and} \qquad a_i^{\pm}(0,x,\theta) = 0 \quad \text{for } i>0\,,$$

where it is understood that $a_{-1}^{\pm}(t,x,\theta) := 0$. For these functions $(*)$ is a telescoping series. The functions satisfy $a_i^{-}(t,x,\theta) = a_i^{+}(-t,x,\theta)$.

Proof. The first order partial differential equations can be solved inductively as follows. Define the two functions

$$a_0^{\pm}(t,x,\theta) := \exp A_{x\pm t\theta/2|\theta|}(\pm t\theta/|\theta|)\,,$$

which are smooth in $(t,x,\theta)\in\mathbb{R}\times\mathbb{R}^n\times\dot{\mathbb{R}}^n$, are positive-homogenous of zeroth order and solve the transport equations $(**)$ with $a_{-1}=0$, as can be easily checked.

Now assume that we have constructed the desired functions up to $a_{N-1}^{\pm}$. Note that $a_0^{\pm}$ is nowhere zero, so that $b_i^{\pm} := a_i^{\pm}/a_0^{\pm}$ is well-defined and smooth, if $a_i^{\pm}$ is. The differential equations $(**)$ for $i>0$ can be rewritten to

$$\pm|\theta|\partial_t b_i^{\pm} - \theta\cdot\operatorname{grad} b_i^{\pm} = \frac{\mathrm{i}}{2a_0^{\pm}}\Box a_{i-1}^{\pm} \qquad \text{with } b_i^{\pm}(0,x,\theta) = 0.$$

Since

$$\frac{\mathrm{d}}{\mathrm{d}t} b_i^{\pm}(\pm|\theta|t, x-t\theta, \theta) = \Big(\pm|\theta|\partial_t b_i^{\pm} - \theta\cdot\operatorname{grad} b_i^{\pm}\Big)(\pm|\theta|t, x-t\theta,\theta)$$

a solution is given by

$$b_i^{\pm}(\pm|\theta|t, x-t\theta,\theta) = \frac{\mathrm{i}}{2}\int_0^t \frac{\Box a_{i-1}^{\pm}}{a_0^{\pm}}(\pm|\theta|\tau, x-\tau\theta,\theta)\,\mathrm{d}\tau$$

and thus changing the parameters gives

$$b_i^{\pm}(t,x,\theta) = \frac{\mathrm{i}}{2}\int_0^{t/\pm|\theta|} \frac{\Box a_{i-1}^{\pm}}{a_0^{\pm}}(\pm|\theta|\tau, x \pm t\theta/|\theta| - \tau\theta, \theta)\,\mathrm{d}\tau$$

A variable substitution in the integral yields

$$a_i^{\pm}(t,x,\theta) = \frac{a_0^{\pm}(t,x,\theta)}{\pm|\theta|}\frac{\mathrm{i}}{2}t\int_0^1 \frac{\Box a_{i-1}^{\pm}}{a_0^{\pm}}(t\tau, x \pm t(1-\tau)\theta/|\theta|, \theta)\,\mathrm{d}\tau\,.$$

With $\Box a_{i-1}^{+}(-t,x,\theta) = \Box a_{i-1}^{-}(t,x,\theta)$ and $a_0^{+}(-t,x,\theta) = a_0^{-}(t,x,\theta)$ it follows that $a_i^{+}(-t,x,\theta) = a_i^{-}(t,x,\theta)$. Further, $\Box a_{i-1}^{\pm}$ is as homogeneous in θ as $a_{i-1}^{\pm}$, which implies inductively that the $a_i^{\pm}$ are indeed positively-homogeneous of degree $-i$. □

With the construction of the functions $a_i^{\pm}$ in the previous proof we obtain the following result, see [GGKW08, Appendix A] for more details.

Remark 4.11. The functions $a_i^{\pm} \in C^\infty(\mathbb{R}\times\mathbb{R}^n\times\dot{\mathbb{R}}^n)$ given by

$$a_0^{\pm}(t,x,\theta) \coloneqq \exp A_{x\pm t\theta/2|\theta|}(\pm t\theta/|\theta|)$$
$$a_i^{\pm}(t,x,\theta) = \frac{a_0^{\pm}(t,x,\theta)}{\pm|\theta|}\frac{\mathrm{i}}{2}t\int_0^1 \frac{\Box a_{i-1}^{\pm}}{a_0^{\pm}}(t\tau, x \pm t(1-\tau)\theta/|\theta|, \theta)\,\mathrm{d}\tau$$

are positive-homogeneous of degree $-i$ in θ and when multiplied with a cut-off function χ, that is zero around 0, we obtain symbols $\chi(|\theta|)a_i^{\pm}(t,x,\theta) \in \mathcal{S}^{-i}$ as in Example 4.4. Let the operators $K_N^{\pm}(t)$ be given by the kernel

$$K_N^{\pm}(t,x,y) = \int_{\mathbb{R}^n} \mathrm{e}^{\mathrm{i}\phi^{\pm}(t,x,y,\theta)}\sum_{i=1}^{N} a_i^{\pm}(t,x,\theta)\chi(|\theta|)\,\mathrm{d}\theta\,.$$

Then $K_N(t) \coloneqq (K_N^{+}(t) + K_N^{-}(t))/2$ approximates the wave operator $K(t)$ in the following sense: Let $u_0 \in C^\infty(\mathbb{R}^n)$ denote some initial data. Since $a_i^{-}(t,x,\theta) = a_i^{+}(-t,x,\theta)$ we have $\partial_{t=0}(a_i^{-} + a_i^{+}) = 0$. Further, $\partial_t\phi^{-} = -\partial_t\phi^{+}$ and thus $K_N(t)$ satisfies the initial condition

$$\partial_{t=0}K_N(t)u_0 = 0\,.$$

Because of the need of a cut-off function we only have

$$K_N(0)u_0 = u_0 + I_0u_0$$

with an integral operator I_0 with smooth kernel. For any $M \in \mathbb{N}$ we have an integral operator I_N with kernel in C^M such that

$$\Box K_N(t)u_0 = I_Nu_0$$

provided $N \in \mathbb{N}$ is sufficiently large. From this it follows that $K(t) - K_N(t)$ is an integral operator with arbitrarily smooth kernel for large N.

We conclude this section by using a so-called "domain of dependence argument" to show that for fixed $t \in \mathbb{R}$ and $y \in \mathbb{R}^n$ the integral kernel $K(t, x, y)$ of the wave operator must have compact support in $x \in \mathbb{R}^n$. The following theorem implies that the speed of the wave propagation is finite and that the solutions to the wave equation are uniquely determined.

Theorem 4.12 (Domain of Dependence).
Let u denote a solution of the wave equation

$$\big(\partial_t^2 + \Delta_a^{\mathrm{D}} + Q\big)u(t,x) = 0 \qquad \text{satisfying the initial conditions}$$
$$u(0,x) = u_0(x) \quad \text{and} \quad \partial_t u(0,x) = u_1(x) \qquad \text{for all } x \in \mathbb{R}^n \text{ and } t \in \mathbb{R}.$$

Fix some point $(t_0, x_0) \in \mathbb{R}^+ \times \mathbb{R}^n$. If the initial values vanish on the *domain of dependence* of (t_0, x_0), that is

$$u_0(x) = u_1(x) = 0 \qquad \text{for all } x \in \mathbb{R}^n \text{ with } |x - x_0| \leq t_0\,,$$

then $u(t_0, x_0) = 0$.

Proof. We give the idea of the argument as presented, for example, in [Vas15, Chapter 7]. Consider the *energy* of the solution u:

$$E(t) \coloneqq \int_{\mathbb{R}^n} |\partial_t u|^2 + |\nabla_{e_i}^{\mathrm{D}} u|^2 + Q|u|^2 \,\mathrm{d}x\,.$$

Differentiating this function by t yields

$$E'(t) = \int_{\mathbb{R}^n} 2\,\mathrm{Re}\Big(\langle \partial_t u, \partial_t^2 u\rangle + \langle \nabla_{e_i}^{\mathrm{D}} \partial_t u, \nabla_{e_i}^{\mathrm{D}} u\rangle + \langle \partial_t u, Qu\rangle\Big)\,\mathrm{d}x\,.$$

If we *assume* that u decays sufficiently fast at infinity we have by integration by parts that

$$E'(t) = \int_{\mathbb{R}^n} 2\,\mathrm{Re}\,\langle \partial_t u, \partial_t^2 u - \nabla_{e_i}^{\mathrm{D}} \nabla_{e_i}^{\mathrm{D}} u + Qu\rangle\,\mathrm{d}x = 0\,.$$

It follows that the energy is an integral of motion.

To show that the speed of the wave propagation is finite one instead considers the function

$$e(t) \coloneqq \int_{|x-x_0| \leq t_0 - t} |\partial_t u|^2 + |\nabla_{e_i}^{\mathrm{D}} u|^2 + Q|u|^2 \,\mathrm{d}x \qquad \text{for } 0 \leq t \leq t_0.$$

Again one differentiates with respect to t but because the domain of integration depends on t this yields boundary terms. Also, the boundary terms of the

integration by parts do not, a priori, vanish. But if one assumes that $Q \geq 0$ then those boundary terms are less than or equal to zero:

$$e'(t) = \int_{|x-x_0|\leq t_0-t} 2\,\mathrm{Re}\langle \partial_t u, (\partial_t^2 + \Delta_a^{\mathrm{D}} + Q)u\rangle \,\mathrm{d}x \;+\; \text{boundary terms} \leq 0$$

Because the initial values vanish on the domain of dependence we have for all $0 \leq t \leq t_0$ that

$$0 \leq e(t) \leq e(0) = 0\,.$$

Again, with $Q \geq 0$ we have, in particular, that $u(t_0, x_0) = 0$.

The general case for arbitrary smooth potentials requires more elaborate estimates. A general result that covers our case can be found in [Tay10, Chapter 2.8]. □

Corollary 4.13. If K is the integral kernel of the wave operator, then the function $x \mapsto K(t, x, y)$ has compact support for all $(t, y) \in \mathbb{R} \times \mathbb{R}^n$.

Proof. If the support of the initial values of the wave equation is a subset of $B_r := \{x \in \mathbb{R}^n \mid |x| \leq r\}$ for some $r > 0$ then the support of the corresponding solution $u(t, \,.\,)$ of the wave equation is a subset of $B_{r+|t|}$ for every fixed $t \geq 0$ by Theorem 4.12. The same is true for $t < 0$ by the symmetry of the wave equation: If u is a solution of the wave equation with $u(0, \,.\,) = u_0$ and $\partial_t u(0, \,.\,) = u_1$ then $v(t, x) := u(-t, x)$ is also a solution but with $\partial_t v(0, \,.\,) = -u_1$.

It follows that $K(t, \,.\,, y)$ has compact support for all $t \in \mathbb{R} \times \mathbb{R}^n$. □

4.3 The Wave Equation on ω

We define the box operator acting on the sections of a nondegenerate line bundle ω as $\Box := \partial_t^2 + \Delta_a^{\mathrm{D}} + Q$. By Remark 1.10 we can identify sections of ω with smooth functions $f \in C^\infty(\mathbb{R}^n)$ that are $\mathcal{L}$-equivariant,

$$f(x + l) = e_l(x) \cdot f(x) \qquad \text{for all } l \in \mathcal{L},$$

recall Definition 1.9.

We define a distributional kernel

$$K_\omega(t, x, y) := \sum_{l \in \mathcal{L}} e_l(x)^{-1} K(t, x + l, y)\,,$$

where $K(t, x, y)$ is the wave kernel associated with $P = \Delta_a^{\mathrm{D}} + Q$ on $\mathbb{R}^n$, and the corresponding wave operator as

$$K_\omega(t)u_0(x) := \int_{\mathcal{F}} K_\omega(t, x, y) u_0(y)\,\mathrm{d}y$$

for all $\mathcal{L}$-equivariant functions u_0 and any fundamental domain $\mathcal{F}$ of the lattice $\mathcal{L}$. As in the case of the heat invariants we could introduce a factor $1/\operatorname{Vol} M$ but to stay in the notation of the appendix of [GGKW08] we will do so later.

The wave operator is well-defined because the sum is finite by Corollary 4.13 and every $K_\omega(t)u_0$ is an $\mathcal{L}$-equivariant function: For any $k \in \mathcal{L}$ we have (with $\mu = k + 1$)

$$\begin{aligned}(K_\omega(t)u_0)(x+k) &= \sum_{l\in\mathcal{L}} e_l(x+k)^{-1} \int_{\mathcal{F}} K(t, x+k+l, y)u_0(y)\,\mathrm{d}y \\ &= e_k(x) \sum_{\mu\in\mathcal{L}} e_\mu(x)^{-1} \int_{\mathcal{F}} K(t, x+\mu, y)u_0(y)\,\mathrm{d}y = e_k(x)K_\omega(t)u_0(x)\,,\end{aligned}$$

because $e_l(k)^{-1} = 1$ and $e_{-k}(x)^{-1} = e_k(x)$.

Further, we have $K(0, x, y) = \delta_x(y)$, where δ_x denotes the Dirac distribution at x. If $k \in \mathcal{L}$ is the lattice vector with $x + k \in \mathcal{F}$ then

$$(K_\omega(0)u_0)(x) = \sum_{l\in\mathcal{L}} e_l(x)^{-1} \int_{\mathcal{F}} \delta_{x+l}(y)u_0(y)\,\mathrm{d}y = e_k(x)^{-1}u_0(x+k) = u_0(x)\,.$$

Thus $K_\omega u_0$ satisfies the first initial condition of the wave equation. The second initial condition is also satisfied because $\partial_{t=0}K = 0$ implies $\partial_{t=0}K_\omega = 0$.

Finally, each connection ∇ on ω must satisfy $\nabla(e_{-l}f(\,.\,+l)) = e_{-l}(\nabla f)(\,.\,+l)$. The same then follows for $\Box$ and it follows that

$$\Box K_\omega(t)u_0 = 0\,.$$

In conclusion, $K_\omega u_0$ is indeed a solution to the wave equation on the sections of the line bundle ω with respect to the differential operator $\Box$.

With this integral kernel $K_\omega(t, x, y)$ of the wave operator K_ω we can write the wave trace as

$$\operatorname{trace} K_\omega(t) = \frac{1}{\operatorname{Vol} M} \int_{\mathcal{F}} K_\omega(t, x, x)\,\mathrm{d}x\,.$$

Recall that we have defined our scalar product on $\mathrm{L}^2(\omega)$ with a normalization factor $1/\operatorname{Vol} M$, confer Definition 3.1. To stay consistent we must include this factor in the wave trace.

By [DG75] the singular support of the wave trace is contained in the set of periods of periodic geodesics of the base manifold M. In our case of flat tori those periods are equal to the lengths of lattice vectors $|\mathcal{L}| := \{\,|l| \mid l \in \mathcal{L}\}$. For any length d let $\beta_d \colon \mathbb{R} \to \mathbb{R}$ denote a smooth function that is 1 near d and whose support is contained in a small interval such that $\operatorname{supp}\beta_d \cap |\mathcal{L}| = \{d\}$. Our aim is to compute the asymptotic expansion of the Fourier transform of the wave trace at $t = d$:

$$(\beta_d \operatorname{trace} K_\omega)\hat{}(\eta) \qquad \text{for } \eta \to \infty.$$

Remark 4.14. By Proposition 4.17 this asymptotic expansion does not depend on the K^--part of the wave kernel and will for this reason only depend on the symbols a_i^+ introduced in Section 4.2.

Definition 4.15. The following definition requires a definition of the *binomial coefficient* that that is valid for a positive and negative $m \in \mathbb{Z}$. We use

$$\binom{m}{k} := \frac{m(m-1)\cdots(m-(k-1))}{k!}\,.$$

Definition 4.16. Let i, k and R denote nonnegative integers. Abbreviate $a_i := a_i^+$ and for $l \in \mathcal{L}\backslash\{0\}$ define, with $\beta_{|l|}$ as above, a smooth function

$$b_{k,l,\beta}\colon \mathbb{R}^n \times S^{n-1} \to \mathbb{C} \qquad \text{by}$$
$$b_{k,l,\beta}(x,\omega) := \sum_{i=0}^{k} \binom{n-1-i}{k-i} \cdot \left(\mathrm{i}\partial_t\right)^{k-i}_{|t=\omega\cdot l} \beta_{|l|}(t) a_i(t, x+l, -\omega)$$

We define a subset of the unit sphere by

$$S^{n-1}_+(l) := \left\{\omega \in S^{n-1} \mid \omega \cdot l > 0\right\}$$

and with the volume element $\mathrm{d}\omega$ of S^{n-1} we set

$$J_{l,R}(\eta) := \frac{1}{(2\pi)^{n-1}} \sum_{k=0}^{R+n-2} \eta^{n-1-k} \int_{\mathcal{F}}\int_{S^{n-1}_+(l)} e_l(x)^{-1} \cdot \mathrm{e}^{-\mathrm{i}\eta\omega l} b_{k,l,\beta}(x,\omega)\,\mathrm{d}\omega\mathrm{d}x\,.$$

With this definition we can expand the wave trace around d in terms of $J_{l,R}$, see [GGKW08, Appendix D]. The proof in [GGKW08] assumes that the length spectrum of M is nondegenerate, i.e. that there are only two lattice vectors $\pm l$ of length d. However, this assumption is not used in the calculation and the following Proposition holds for all (even-dimensional) lattices $\mathcal{L}$.

Proposition 4.17. For $d \in |\mathcal{L}|\backslash\{0\}$ and $R \in \mathbb{N}$

$$(\beta_d \operatorname{trace} K_\omega)\hat{}\,(\eta) = \frac{1}{2\operatorname{Vol} M} \sum_{|l|=d} J_{l,R}(\eta) + O(\eta^{-R}) \qquad \text{for } \eta \to \infty.$$

The $J_{l,R}$ are constructed from the symbols $a_i := a_i^+$ of K^+. The contribution of K^- to the asymptotic expansion of the wave trace is in $O(\eta^{-\infty})$.

We can now proceed to compute an asymptotic expansion of $J_{l,R}(\eta)$ by applying the method of stationary phase as described in, for example, [GS94, Section 2] to the integral

$$\int_{S^{n-1}_+(l)} \mathrm{e}^{-\mathrm{i}\eta\omega l} b_{k,l,\beta}(x,\omega)\,\mathrm{d}\omega\,.$$

The map $S^{n-1}_+(l) \ni \omega \mapsto -\omega l \in \mathbb{R}$ has exactly one critical point at $l/|l|$ and this critical point is a minimum. We will construct Morse coordinates around this point. Those coordinates are given in [GGKW08, Lemma C.3] but we are more specific about the volume form here, which allows us to compute higher wave invariants later.

Lemma 4.18. Let $B^{n-1}_{\sqrt{2}}(0)$ denote the ball of radius $\sqrt{2}$ in $\mathbb{R}^{n-1}$. The map

$$y\colon B^{n-1}_{\sqrt{2}}(0) \to S^{n-1}_+(e_n) \qquad \text{with}$$
$$y(z) \coloneqq \Big(\frac{z}{\kappa(z)}, 1 - \frac{|z|^2}{2}\Big) \qquad \text{and} \qquad \kappa(z) \coloneqq \Big(1 - \frac{|z|^2}{4}\Big)^{-1/2}$$

defines coordinates on $S^{n-1}_+(e_n)$. Let R_l denote an orthogonal linear map that maps e_n onto $l/|l|$ and define coordinates for $S^{n-1}_+(l)$ by

$$\omega(z) \coloneqq R_l(y(z))\,.$$

In these coordinates we have

(i) $\omega(z) \cdot l/|l| = 1 - |z|^2/2$ and

(ii) the volume element on $S^{n-1}_+(l)$ is given by $v(z)\mathrm{d}z$ with $v(z) = \kappa(z)^{3-n}$.

Proof. The map y is clearly well-defined, smooth and has the smooth inverse

$$S^{n-1}_+(e_n) \ni y \mapsto \sqrt{\frac{2}{1+y_n}}(y_1, \dots, y_{n-1}) \in B_{\sqrt{2}}\,.$$

It is thus a diffeomorphism and defines coordinates.

Claim (i) is easy to show:

$$\omega(z) \cdot l/|l| = y(z) \cdot R_l^{-1} l/|l| = y(z) \cdot e_n = 1 - |z|^2/2\,.$$

It remains to compute the volume element in the z-coordinates. If (x_i) denote the standard coordinates of $\mathbb{R}^n$ then the the map

$$(x_1, \dots, x_{n-1}) \mapsto (x_1, \dots, x_{n-1}, \sqrt{1 - x_1^2 - \dots - x_{n-1}^2})$$

gives coordinates on $S^{n-1}_+(e_n)$ and the volume element in these coordinates is given by

$$\frac{1}{x_n}\mathrm{d}x \qquad \text{with } x_n = \sqrt{1 - x_1^2 - \dots - x_{n-1}^2}.$$

Define $\psi(z) \coloneqq z/\kappa(z)$. For every $w \perp z$ we have $\mathrm{d}\psi_z \cdot w = \frac{1}{\kappa(z)} \cdot w$ and further

$$\mathrm{d}\psi_z \cdot z = \partial_{t=1} \frac{tz}{\kappa(tz)} = \frac{z}{\kappa(z)} - \frac{\kappa(z)}{4}|z|^2 \cdot z = \kappa(z) \cdot \Big(\frac{1}{\kappa(z)^2} - \frac{1}{4}|z|^2\Big) \cdot z\,.$$

With $\frac{1}{\kappa(z)^2} - \frac{1}{4}|z|^2 = 1 - \frac{1}{2}|z|^2 = x_n$ it follows that

$$|\det \mathrm{d}\psi_z| = \frac{1}{\kappa(z)^{n-2}} \cdot \kappa(z) \cdot x_n = \kappa(z)^{3-n} \cdot x_n$$

and the claim follows. □

More details about the coordinates $\omega(z)$, in particular their derivatives at $z = 0$, can be found in Appendix A.

With the Morse coordinates z we can rewrite the integral as follows:

$$\int_{S^{n-1}_+(l)} \mathrm{e}^{-\mathrm{i}\eta\omega l} b_{k,l,\beta}(x,\omega)\,\mathrm{d}\omega = \int_{B_{\sqrt{2}}} \mathrm{e}^{-\mathrm{i}\eta|l|(1-|z|^2/2)} b_{k,l,\beta}(x,\omega(z))v(z)\,\mathrm{d}z$$

We write $\Delta_z \coloneqq \partial^2_{z_1} + \cdots + \partial^2_{z_{n-1}}$. Note that this is not the sign convention used for Δ^{D}_a. With the method of stationary phase we have by [GS94, (2.6) page 21] that for any $N \in \mathbb{N}$

$$\begin{aligned}\int_{S^{n-1}_+(l)} &\mathrm{e}^{-\mathrm{i}\eta\omega l} b_{k,l,\beta}(x,\omega)\,\mathrm{d}\omega \\ &= \mathrm{e}^{-\mathrm{i}\eta|l|} \sum_{j=0}^{N-1} \frac{(2\pi)^{\frac{n-1}{2}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}(n-1)}}{j!(|l|\eta)^{j+\frac{n-1}{2}}(-2\mathrm{i})^j} \Delta^j_{z=0} b_{k,l,\beta}(x,\omega(z))v(z) + O(\eta^{-N-\frac{n-1}{2}})\end{aligned}$$

for $\eta \to \infty$. In particular, this asymptotic expansion only depends on $b_{k,l,\beta}(x,\omega(z))$ in a small neighborhood of $z = 0$ or equivalently on $b_{k,l,\beta}(x,\omega)$ in a small neighborhood of $l/|l|$. Since $\beta(\omega l)$ is identical to 1 on a sufficiently small neighborhood of $l/|l|$ we can henceforth assume that $\beta \equiv 1$ and drop it from our notation, just as it is done in [GGKW08].

Remark 4.19. There is a sign error in [GGKW08, page 2489] in the corresponding expansion following equation (C.10). In the expansion given in [GS94, equation (2.6)] there is the term $\langle D_x, Q^{-1}D_x\rangle^k$, where we have $Q = |l|\mathbb{E}_{n-1}$ here. In this term the derivatives D_x have been replaced by ∂_z. However, in the notation of [GS94] $D_x = \frac{1}{\mathrm{i}}\partial_x$ and thus we need to replace

$$\langle D_x, Q^{-1}D_x\rangle^k \qquad \text{not by} \qquad (\Delta_z/|l|)^k \qquad \text{but by} \qquad (-\Delta_z/|l|)^k\,.$$

This sign error is significant: Computing the wave invariant without the minus sign will lead to expressions violating, for example, the necessary condition given in Lemma 4.37 below. However, since the wave invariants have been computed only partially in [GGKW08] this error has no effect on their final results.

We can now combine the expansion of the wave trace in terms of $J_{l,R}(\eta)$ and the expansion of $J_{l,R}(\eta)$ by the method of stationary phase to obtain an expansion of the wave trace with computable coefficients, coefficients which we will call wave invariants as in [GGKW08]. Recall that

$$J_{l,R}(\eta) \coloneqq \frac{1}{(2\pi)^{n-1}} \sum_{k=0}^{R+n-2} \eta^{n-1-k} \int_{\mathcal{F}} \int_{S_+^{n-1}(l)} e_l(x)^{-1} \cdot \mathrm{e}^{-\mathrm{i}\eta\omega l} b_{k,l,\beta}(x,\omega)\, \mathrm{d}\omega \mathrm{d}x\,.$$

It follows that

$$\begin{aligned} J_{l,R}(\eta) = \frac{\mathrm{e}^{-\mathrm{i}\eta|l|}}{(2\pi)^{n-1}} \sum_{k=0}^{R+n-2} \eta^{n-1-k} \int_{\mathcal{F}} e_l(x)^{-1} \\ \sum_{j=0}^{N_k-1} \frac{(2\pi)^{\frac{n-1}{2}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}(n-1)}}{j!(|l|\eta)^{j+\frac{n-1}{2}}(-2\mathrm{i})^j} \Delta_{z=0}^j b_{k,l}(x,\omega(z))v(z) + O(\eta^{-N_k-\frac{n-1}{2}})\, \mathrm{d}x \end{aligned}$$

for $\eta \to \infty$. We choose the summation limits $N_k - 1$ so that the error terms are of order $O(\eta^{-R})$. We need for $\eta > 1$ that

$$\eta^{n-1-k} \cdot \eta^{-N_k-\frac{n-1}{2}} \le \eta^{-R} \qquad \text{which means} \qquad N_k \ge R + \frac{n-1}{2} - k\,.$$

It is convenient to use a bigger than necessary summation limit (and a nonnegative one), let $N_k \coloneqq R + n - 1 - k > R + \frac{n-1}{2} - k$. Thus,

$$\begin{aligned} J_{l,R}(\eta) = \frac{\mathrm{e}^{-\mathrm{i}\eta|l|}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}(n-1)}}{(2\pi|l|)^{\frac{n-1}{2}}} \sum_{k=0}^{R+n-2} \eta^{\frac{n-1}{2}} \sum_{j=0}^{R+n-2-k} \frac{1}{\eta^{k+j}} \int_{\mathcal{F}} e_l(x)^{-1} \\ \frac{1}{j!|l|^j(-2\mathrm{i})^j} \Delta_{z=0}^j b_{k,l}(x,\omega(z))v(z)\, \mathrm{d}x + O(\eta^{-R}) \end{aligned}$$

We regroup those two sums and order this expansion by order of η. With

$$C_{|l|}(\eta) \coloneqq \frac{\mathrm{e}^{-\mathrm{i}\eta|l|}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}(n-1)}}{(2\pi|l|)^{\frac{n-1}{2}}} \cdot \eta^{\frac{n-1}{2}}$$

we can write

$$J_{l,R}(\eta) = C_{|l|}(\eta) \sum_{s=0}^{R+n-2} \sum_{j=0}^{s} \frac{1}{\eta^s} \int_{\mathcal{F}} e_l(x)^{-1} \frac{1}{j!(-2\mathrm{i}|l|)^j} \Delta_{z=0}^{j} b_{s-j,l}(x, \omega(z)) v(z) \, \mathrm{d}x + \mathcal{O}(\eta^{-R}) .$$

As in [GGKW08, Appendix C] we can now set

$$C_k(x,l) \coloneqq \sum_{j=0}^{k} \frac{1}{j!} \frac{1}{(-2\mathrm{i}|l|)^j} e_l(x)^{-1} \Delta_{z=0}^{j} b_{k-j,l}(x, \omega(z)) v(z)$$

and have an asymptotic expansion not just of $J_{l,R}(\eta)$ but, by Proposition 4.17, of the wave trace at $d \in |\mathcal{L}| \setminus \{0\}$:

$$(\beta_d \operatorname{trace} K_\omega)\hat{}(\eta) \sim \frac{1}{2 \operatorname{Vol} M} C_d(\eta) \sum_{k=0}^{\infty} \frac{1}{\eta^k} \cdot \sum_{|l|=d} \int_{\mathcal{F}} C_k(x,l) \, \mathrm{d}x$$

for $\eta \to \infty$.

Because $(\beta_d \operatorname{trace} K_\omega)\hat{}$ is determined by the spectrum of $\Delta_a^{\mathrm{D}} + Q$ it follows that each coefficient

$$\frac{1}{\operatorname{Vol} M} \sum_{|l|=d} \int_{\mathcal{F}} C_k(x,l) \, \mathrm{d}x$$

is also spectrally determined.

Before concluding this section it is convenient to reformulate the wave invariants and bring them into a form more suitable for computations. We begin with some observations about the structure of the formulas describing the wave invariants.

We first consider the symbols a_i used to construct the $b_{k,l}$ in Definition 4.16.

Remark 4.20. The symbols $a_i \coloneqq a_i^+$ were given in Remark 4.11 as

$$a_0(t,x,\theta) \coloneqq \exp A_{x+t\theta/2|\theta|}(t\theta/|\theta|) \qquad \text{and}$$
$$a_i(t,x,\theta) = \frac{a_0(t,x,\theta)}{|\theta|} \frac{\mathrm{i}}{2} t \int_0^1 \frac{\Box a_{i-1}}{a_0}(t\tau, x + t(1-\tau)\theta/|\theta|, \theta) \, \mathrm{d}\tau .$$

The only source of exponential terms in a_i is a_0. It follows inductively that we can write each symbol in the form

$$a_i = a_0 \frac{\mathrm{i}}{2} t A_i ,$$

where A_i is a polynomial in A^{D}, $\tilde{a}$ and Q (with integrals over τ-variables) that is free of any exponential terms:

To obtain a_{i+1} from $a_i = a_0 \frac{\mathrm{i}}{2} t A_i$ we have to apply the differential operator $\Box = \partial_t^2 + \Delta_a^{\mathrm{D}} + Q$ to a_i. The derivatives in $\Box$ either "pull down" terms from a_0 or they are applied to $\frac{\mathrm{i}}{2} t A_i$. In both cases we obtain an expression where every summand has exactly one factor a_0. The factor a_0 is removed by $\frac{1}{a_0}$ under the τ-integral. Applying the integral then gives A_{i+1}, which is again of the desired form.

A similar argument allows us to track the exponential terms of the wave invariants and provides the following definition.

Definition 4.21. We rewrite $C_k(x,l)$ by inserting the definition of $b_{k-j,l}$.

$$\begin{aligned} C_k(x,l) &= \sum_{j=0}^{k} \frac{e_l(x)^{-1}}{j!(-2\mathrm{i}|l|)^j} \Delta_{z=0}^{j} v(z) \sum_{i=0}^{k-j} \tbinom{n-1-i}{k-i-j} (\mathrm{i}\partial_t)^{k-i-j}_{t=\omega(z)\cdot l} a_i(t, x+l, -\omega(z)) \\ &= \sum_{i+j\le k} \frac{e_l(x)^{-1}}{j!(-2\mathrm{i}|l|)^j} \tbinom{n-1-i}{k-i-j} \Delta_{z=0}^{j} v(z) (\mathrm{i}\partial_t)^{k-i-j}_{t=\omega(z)\cdot l} a_i(t, x+l, -\omega(z)) \end{aligned}$$

We have by Remark 4.20 that $a_i = a_0 \frac{\mathrm{i}}{2} t A_i$. The ∂_t-derivatives and, after the substitution of arguments $(t,x,\omega) \mapsto (t, x+l, -\omega(z))$, the z-Laplacian again "pull down" more terms from the exponential a_0 and leave exactly one exponential factor, namely a_0, within each obtained summand. We can factor this exponential term, together with $e_l(x)^{-1}$, and write the wave invariants as follows:

$$\begin{aligned} C_k(x,l) &= e_l(x)^{-1} a_0(\omega(0)\cdot l, x+l, -\omega(0)) \sum_{i+j\le k} H(i,j,k)(x) \\ &= e_l(x)^{-1} a_0(|l|, x+l, -l/|l|) \cdot \sum_{i+j\le k} H(i,j,k)(x) \end{aligned}$$

Here we *define* $H(i,j,k)$ as the expression obtained by first performing all derivations associated to the triple (i,j,k) and then removing all remaining factors $\exp(\cdot)$.

To calculate the wave invariants we simplify the exp-factors not included in $H(i,j,k)$.

Definition 4.22. The signature of a lattice vector $l \in \mathcal{L}$ shall be defined as

$$\sigma_l := e_l(l/2) \in \{\pm 1\}\,.$$

The definition of $e_x(y)$ is given in Definition 1.9. We have $e_l(l/2) = \pm 1$, depending on the Chern invariant factors $(r_1, \dots, r_m)$ and the chosen lattice vector $l \in \mathcal{L}$.

Recall that $E_a(l) \coloneqq \mathrm{e}^{-\tilde{a}(l)}$ by Definition 2.2 and that $Fl \coloneqq F(l, .) \in \mathbb{R}^{n\prime}$ by Definition 2.5.

Lemma 4.23. $e_l(x)^{-1} a_0(|l|, x + l, -l/|l|) = E_{Fl}(x) E_a(l) \sigma_l$

Proof. The function $a_0 = a_0^+$ is given in Remark 4.11. Additionally, we use

$$\tilde{F}(X, Y) = A_Y^{\mathrm{D}}(X) - A_X^{\mathrm{D}}(Y)$$

as given in Lemma 1.15.

$$\begin{aligned} &e_l(x)^{-1} a_0(|l|, x + l, -l/|l|) = \exp(-2\pi \mathrm{i} w_l(x) + A_{x+l-l/2}(-l)) \\ &= \exp(A_l^{\mathrm{D}}(x) - A_x^{\mathrm{D}}(l) - A_l^{\mathrm{D}}(l/2) - \tilde{a}(l)) \\ &= \exp(\tilde{F}(x, l) + 2\pi \mathrm{i} w_l(l/2) - \tilde{a}(l)) \\ &\qquad = \exp(-\tilde{F}(l)(x)) e_l(l/2) E_a(l) = E_{Fl}(x) \sigma_l E_a(l) \,. \end{aligned}$$ □

Combining the results of this and the previous discussion, we have the following spectral invariants of $\Delta_a^{\mathrm{D}} + Q$.

Theorem 4.24 (Wave Invariants).
For every even-dimensional flat torus $M = \mathbb{R}^n / \mathcal{L}$ given by some lattice $\mathcal{L}$, every Hermitian line bundle ω given by some nondegenerate 2-form F, every translation-invariant connection $a \in \mathbb{R}^{n\prime}$ and every potential Q we define the *partial wave invariants* by

$$\mathsf{WI}_{k,l}(a, Q) \coloneqq \sum_{i+j \le k} \langle H(i, j, k), E_{-Fl} \rangle \,.$$

The *wave invariants* defined by

$$\mathsf{WI}_{k,d}(a, Q) \coloneqq \sum_{|l|=d} E_a(l) \sigma_l \mathsf{WI}_{k,l}(a, Q)$$

are spectral invariants of $\Delta_a^{\mathrm{D}} + Q$ for every $k \in \mathbb{N}$ and every $d \in |\mathcal{L}| \backslash \{0\}$.

4.4 The Recipe

Before continuing to compute the wave invariants given in Theorem 4.24 we give a retrospective summary of all definitions leading to the wave invariants. This section contains a description, a recipe, of how the wave invariants of the Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$ for some connection $a \in \mathbb{R}^{n'}$ and a smooth potential on an even-dimensional torus M can be computed.

The torus $M \coloneqq \mathbb{R}^n/\mathcal{L}$ is given by a lattice $\mathcal{L}$ and the connection $a \in \mathbb{R}^{n'}$ acts on sections of the line bundle ω and has the curvature form $-\tilde{F}$, where $\tilde{F} \coloneqq 2\pi\mathrm{i}F$. With $n = 2m$ there is a Chern basis $\{U_1, \dots, U_m, V_1, \dots, V_m\}$ of the lattice $\mathcal{L}$ such that

$$F\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \qquad \text{satisfies } F(U_i, V_j) = r_i \delta_{ij}$$

with natural numbers, the Chern invariant factors, $r_1 | \cdots | r_m$. With the coordinates $(u^1, \dots, u^m, v^1, \dots, v^m)$ of the Chern basis we define

$$w_x(y) \coloneqq \sum_{i=1}^{m} r_i u^i(x) v^i(y) \qquad \text{and} \qquad A_x^{\mathrm{D}} \coloneqq -\tilde{w}_x$$

such that $A_x \coloneqq A_x^{\mathrm{D}} + \tilde{a}$ is the connection form of the connection a.

In Remark 4.11 we have constructed symbols that give, when summed, an approximation to the wave kernel on $\mathbb{R}^n$. We only need $a_i \coloneqq a_i^+$ and we only need these functions for $\omega \in S^{n-1}$. They are defined as

$$\begin{aligned} a_0(t, x, \omega) &= \exp\Big(A_{x+t\omega/2}(t\omega)\Big) \\ a_i(t, x, \omega) &= a_0(t, x, \omega) \cdot \frac{\mathrm{i}}{2} t \int_0^1 \frac{\Box a_{i-1}}{a_0}(\tau_i t, x + (1-\tau_i)t\omega, \omega)\, \mathrm{d}\tau_i \,, \end{aligned}$$

where

$$\Box = \partial_t^2 - \operatorname{div} \circ \operatorname{grad} - \operatorname{div} A^{\#} - 2A \circ \operatorname{grad} + \|A\|^2 + Q$$

is the wave operator of the Schrödinger operator given by the connection form A and the potential Q, recall Proposition 1.35. The index i of the integration variable τ_i will be helpful later on.

In Lemma 4.18 we have constructed Morse coordinates and computed the volume form in those coordinates. They are given by

$$\begin{aligned} &\omega\colon B^{n-1}_{\sqrt{2}}(0) \to \mathbb{R}^n \qquad \text{and} \qquad v\colon B^{n-1}_{\sqrt{2}}(0) \to \mathbb{R} \qquad \text{with} \\ &v(z) = \kappa(z)^{3-n} \qquad \text{and} \qquad \omega(z) = R_l\Big(\frac{z}{\kappa(z)}, 1 - \frac{1}{2}|z|^2\Big) \end{aligned}$$

where $\kappa(z) = (1 - |z|^2/4)^{-1/2}$ and R_l is an orthogonal linear map with $R_l e_n = l/|l|$. We define an orthonormal basis $\{W_1, \dots, W_{n-1}, l/|l|\}$ of $\mathbb{R}^n$ by $R_l(e_i) = W_i$ for $i = 1, \dots, n-1$.

We have expanded the wave trace in terms of the symbols a_i using the Morse coordinates above. For every $k \in \mathbb{N}$ and $i, j \geq 0$ with $i + j \leq k$ and some fixed nonzero lattice vector $l \in \mathcal{L}\backslash\{0\}$ we define

$$H(i,j,k)(x) = \frac{\binom{n-1-i}{k-i-j}}{j!(-2\mathrm{i}|l|)^j} \Delta_{z=0}^{j} v(z) (\mathrm{i}\partial_t)_{t=\omega(z)\cdot l}^{k-i-j} a_i(t, x+l, -\omega(z)) \\ \texttt{/.Exp[\_]->1},$$

where f `/.Exp[_]->1` means, following MATHEMATICA notation, that all exponential terms in the expression f are set to 1, see Remark 4.20 and Definition 4.21.

Further, recall that $E_c := \mathrm{e}^{-\tilde{c}}$ and that $Fl = F(l, .) \in \mathcal{L}'$. For $k \in \mathbb{N}$ and $l \in \mathcal{L}\backslash\{0\}$ the *partial wave invariants* are defined as

$$\mathsf{WI}_{k,l}(a, Q) := \sum_{i+j\leq k} \langle H(i,j,k), E_{-Fl} \rangle$$

and, by Theorem 4.24, for each $d \in |\mathcal{L}|\backslash\{0\}$

$$\mathsf{WI}_{k,d}(a, Q) := \sum_{|l|=d} E_a(l) \sigma_l \mathsf{WI}_{k,l}(a, Q)$$

(with $\sigma_l := e_l(l/2) = \mathrm{e}^{\tilde{w}_l(l)/2} \in \{\pm 1\}$) is a spectral invariant of $\Delta_a^{\mathrm{D}} + Q$. The $\mathsf{WI}_{k,d}(a, Q)$ are called the *wave invariants* of (ω, M, a, Q).

The aim of the following sections is to find general properties of those wave invariants, compute the first wave invariants using this recipe and use those invariants to obtain isospectrality results.

4.5 The First Wave Invariant

4.5.1 Calculation of a_1

We will start our study of the wave invariants by calculating the first of those invariants. In principle, the algorithm given in Section 4.4 provides us with a method to compute all wave invariants using only elementary operations: derivation of polynomials and one exponential, substitution of arguments and simple integrations. However, the involved expressions will very rapidly increase in size when considering higher invariants.

The aim of this and the following sections is therefore not only to compute the first and second wave invariant, but also to find abbreviations that

satisfy three criteria: They shorten the involved expressions, they preserve the mathematical content of those expressions and they can be used for an automated computation of the higher wave invariants in Appendix D.

We will call such an abbreviation a *notation*. The computation of the first two wave invariants by hand serves to illustrates the function of the notations.

The first idea is to use the *Einstein summation convention* not only for different sums, but also for integrals.

Notation 4.25 (Einstein convention and traces).
Each summand S of the wave invariants that contains any of the terms x_i, e_i or W_i is understood to be summed over. However, there are two different ranges of summation:

- Summands containing x_i or e_i or a combination thereof are summed over the index set $i \in \{1, \dots, n\}$,

$$S(\partial_{x_i}, e_i) \coloneqq \sum_{i=1}^{n} S(\partial_{x_i}, e_i)\,.$$

- Summands containing ∂_{z_i} or W_i or a combination thereof are summed over the index set $i \in \{1, \dots, n-1\}$,

$$S(\partial_{z_i}, W_i) \coloneqq \sum_{i=1}^{n-1} S(\partial_{z_i}, W_i)\,.$$

Note that in the following calculations we will use the term x_i only as an argument of ∂. For dependencies of the form, say, $x \mapsto A^{\mathrm{D}}_x(\omega)$ we will always use the term "x". Furthermore, if there is such a dependency we will always write this "x" explicitly. If a term contains a bilinear function without arguments those "open slots" are understood to contain e_i's. For example $A^{\mathrm{D}}_\omega A^{\mathrm{D}}(\omega)$ stands for $A^{\mathrm{D}}_\omega(e_i)A^{\mathrm{D}}_{e_i}(\omega)$ and $\tilde{a}A^{\mathrm{D}}(\omega)$ represents $\tilde{a}(e_i)A^{\mathrm{D}}_{e_i}(\omega)$. Of course, only one such abbreviation can be used per summand.

The e_i always appear in pairs within each summand and thus the latter notation is an abbreviation for *traces* of bilinear maps, for example

$$A^{\mathrm{D}2}_x = A^{\mathrm{D}}_x(e_i)^2 = \operatorname{Tr} A^{\mathrm{D}}_x \cdot A^{\mathrm{D}}_x\,.$$

The value of a trace of a bilinear map is independent of the orthonormal basis used to evaluate it and in the calculation of wave invariants there are two different such bases in use: The standard basis $\{e_1, \dots, e_n\}$ and $\{W_1, \dots, W_{n-1}, l/|l|\}$. This means that we can switch from using one basis to using the other. To point to such a change of basis we use the notation

$$S(e_i, e_i) \overset{e_i}{=} S(W_i, W_i) + S(l, l)/|l|^2\,,$$

where S is bilinear.

Note however, that the W_i may appear in higher than quadratic order and in this case we cannot substitute the $\{W_i, l/|l|\}$ by the standard basis $\{e_i\}$. The $\{e_i\}$, on the other hand, will always appear in quadratic order. We can always switch from using $\{e_i\}$ to using $\{W_i, l/|l|\}$.

Notation 4.26 (Einstein convention for integrals).
Every τ_i-variable that appears in the calculation of the wave invariants is integrated over the interval $[0,1]$. In the same spirit as the summation over indices is dropped by the Einstein summation convention those integrals shall be omitted,

$$S(\tau_1,\dots,\tau_k) \coloneqq \int_{[0,1]^k} S(\tau_1,\dots,\tau_k)\,\mathrm{d}\tau_1\cdots\mathrm{d}\tau_k\,.$$

The various terms in the calculation of the wave invariants will contain different numbers of τ-variables and are thus integrated over different domains. Since each variable τ_i is always integrated over $[0,1]$ this ambiguity does not lead to errors.

We will use the symbol "$\overset{\tau}{=}$" to remind the reader of this abbreviation. For example,

$$-A^{\mathrm{D}}_{e_i}(t\tau_1\omega)^2 \overset{\tau}{=} -\frac{1}{3}t^2 A^{\mathrm{D}}_{e_i}(\omega)^2\,.$$

With those two notations we can rewrite the definition of the symbols a_i with $i>1$ from Section 4.4 as

$$a_i(t,x,\omega) \overset{\tau}{=} a_0(t,x,\omega)\cdot\frac{\mathrm{i}}{2}t\frac{\Box a_{i-1}}{a_0}(\tau_i t, x+(1-\tau_i)t\omega,\omega)\,.$$

There are two more things to shorten here through notations.

Notation 4.27 (Substitution of variables).
In the calculation of a_i we need to substitute the variables

$$(t,x,\omega) \qquad \text{by} \qquad (t\tau_i, x+(1-\tau_i)t\omega,\omega)\,.$$

This substitution shall be denoted by

$$S(t,x,\omega) \to_i T(t,x,\omega,\tau_i) \qquad \text{if } T(t,x,\omega,\tau_i) = S(t\tau_i, x+(1-\tau_i)t\omega,\omega)\,.$$

We will drop the variables (t,x,ω) and write

$$a_i = a_0\frac{\mathrm{i}}{2}t\cdot A_i \qquad \text{where} \qquad \frac{\Box a_{i-1}}{a_0} \to_i A_i\,,$$

confer Remark 4.20.

The exponential terms in the wave invariants and in the calculation thereof are rather simple and can thus be frequently omitted from the notation. Recall Remark 4.20 and Definition 4.21: The only source of exponential terms in a_i and more generally $H(i,j,k)$ is a_0. In particular, all symbols satisfy $a_i = a_0 \frac{\mathrm{i}}{2} t A_i$ with A_i a polynomial in A^{D}, $\tilde{a}$ and Q. A_i is free of any exponential terms. Those polynomials are generated by applying the differential operator $\Box$ repeatedly. Similarly, the z-Laplacian and the ∂_t-derivative in the definition of H "pull down" more terms from the exponential a_0. After the application of all derivatives all exponential terms are removed, see Definition 4.21.

Notation 4.28. Different summands in the computation of a_i and H have different numbers of derivatives and we want to remove exponential terms as soon as possible. Thus, we write $S \overset{a_0}{=} T$ if $S = a_0 \cdot T$ holds. Additionally, if $S \overset{a_0}{=} T$ and R is some other term then we set $S + R \overset{a_0}{=} T + R$. In other words, dropping exponential terms from some but not all summands of a sum is allowed in this notation.

We can use the notation "$\overset{a_0}{=}$" after all derivatives of $\Box a_{i-1}$ in the definition of A_i have been computed and then again after all derivatives of $H(i,j,k)$ have been computed. We remove a_0 as soon as possible but no sooner.

Both for the first and the second wave invariant we need an explicit expression of a_1 and we have enough notations to compute A_1.

$$a_i(t,x,\omega) \overset{\text{Def}}{=} a_0(t,x,\omega)\frac{\mathrm{i}}{2} t \cdot A_i(t,x,\omega) \qquad \text{with} \qquad \frac{\Box a_{i-1}}{a_0} \to_i A_i$$
$$\text{and} \qquad a_0(t,x,\omega) = \exp(A_{x+t\omega/2}(t\omega))\,.$$

By Proposition 1.35 the wave operator $\Box$ can be written as

$$\Box = \partial_t^2 - \partial_{x_i}^2 - A^{\mathrm{D}}_{e_i}(e_i) - 2A_x(e_i)\partial_{x_i} - A_x(e_i)^2 + Q(x)$$

in standard coordinates. We now calculate each of the six terms of $\Box a_0$ separately using the notations introduced above.

$$\begin{aligned}\partial_t^2 a_0 &= \partial_t(a_0 \cdot (A_{x+t\omega/2}(\omega) + tA^{\mathrm{D}}_{\omega/2}(\omega))) = \partial_t(a_0 \cdot (A_{x+t\omega}(\omega))) \\ &\overset{a_0}{=} (A_{x+t\omega}(\omega))^2 + A^{\mathrm{D}}_{\omega}(\omega) \\ &\to_1 (A_{x+(1-\tau_1)t\omega+t\tau_1\omega}(\omega))^2 + A^{\mathrm{D}}_{\omega}(\omega) \overset{\tau}{=} A_{x+t\omega}(\omega)^2 + A^{\mathrm{D}}_{\omega}(\omega)\end{aligned}$$

$$\begin{aligned}-\partial_{x_i}^2 a_0 &= -\partial_{x_i}(a_0 \cdot A^{\mathrm{D}}_{e_i}(t\omega)) \overset{a_0}{=} -A^{\mathrm{D}}_{e_i}(t\omega)^2 \\ &\to_1 -A^{\mathrm{D}}_{e_i}(t\tau_1\omega)^2 \overset{\tau}{=} -\frac{1}{3}t^2 A^{\mathrm{D}}_{e_i}(\omega)^2 = -\frac{1}{3}t^2 A^{\mathrm{D}}(\omega)^2\end{aligned}$$

$$-A^{\mathrm{D}}_{e_i}(e_i)a_0 \overset{a_0}{=} -A^{\mathrm{D}}_{e_i}(e_i) \to_1 -A^{\mathrm{D}}_{e_i}(e_i) = -A^{\mathrm{D}} \overset{\tau}{=} -A^{\mathrm{D}}$$

$$\begin{aligned}-2A_x(e_i)\partial_{x_i}a_0 &\overset{a_0}{=} -2A_x(e_i)A^{\mathrm{D}}_{e_i}(t\omega) \to_1 -2A_{x+(1-\tau_1)t\omega}(e_i)A^{\mathrm{D}}_{e_i}(\omega)t\tau_1\\ &\overset{\tau}{=} -A_{x+t\omega}A^{\mathrm{D}}(\omega)t + \frac{2}{3}t^2A^{\mathrm{D}}_\omega A^{\mathrm{D}}(\omega)\end{aligned}$$

$$\begin{aligned}-A_x(e_i)^2a_0 &\overset{a_0}{=} -A_x(e_i) \to_1 -A_{x+(1-\tau_1)t\omega}(e_i)^2 = -(A_{x+t\omega}(e_i) - A^{\mathrm{D}}_\omega(e_i)\tau_1 t)^2\\ &\overset{\tau}{=} -A_{x+t\omega}(e_i)^2 + A_{x+t\omega}(e_i)A^{\mathrm{D}}_\omega(e_i)t - \frac{1}{3}A^{\mathrm{D}}_\omega(e_i)^2t^2\\ &= -A^2_{x+t\omega} + A_{x+t\omega}A^{\mathrm{D}}_\omega t - \frac{1}{3}{A^{\mathrm{D}}_\omega}^2t^2\end{aligned}$$

$$Q(x)a_0 \overset{a_0}{=} Q(x) \to_1 Q(x + (1-\tau_1)t\omega)$$

Adding all those terms gives A_1:

$$\begin{aligned}A_1 = {}& A^{\mathrm{D}}_x(\omega)^2 + 2tA^{\mathrm{D}}_x(\omega)A^{\mathrm{D}}_\omega(\omega) + 2\tilde{a}(\omega)A^{\mathrm{D}}_x(\omega) + t^2A^{\mathrm{D}}_\omega(\omega)^2 + 2t\tilde{a}(\omega)A^{\mathrm{D}}_\omega(\omega)\\ &+ \tilde{a}(\omega)^2 + A^{\mathrm{D}}_\omega(\omega) - \frac{1}{3}t^2A^{\mathrm{D}}(\omega)^2 - A^{\mathrm{D}} - A^{\mathrm{D}}_xA^{\mathrm{D}}(\omega)t - \frac{1}{3}A^{\mathrm{D}}_\omega A^{\mathrm{D}}(\omega)t^2\\ &- \tilde{a}A^{\mathrm{D}}(\omega)t - {A^{\mathrm{D}}_x}^2 - tA^{\mathrm{D}}_xA^{\mathrm{D}}_\omega - 2\tilde{a}A^{\mathrm{D}}_x - t\tilde{a}A^{\mathrm{D}}_\omega - \tilde{a}^2 - \frac{1}{3}{A^{\mathrm{D}}_\omega}^2t^2\\ &+ Q(x + (1-\tau_1)t\omega)\end{aligned}$$

The calculation of a_2 or, equivalently, A_2 can be done in the same way. However, A_2 consists of 696 summands! Thus, a straightforward calculation will not be practical. We will continue with the computation of $\mathsf{WI}_{1,d}(a, Q)$ and compute the second wave invariant later with more notations that will reduce size of intermediate expressions.

4.5.2 Calculation of $\mathsf{WI}_{1,d}$

To compute the first wave invariant we need to know all $H(i,j,k)$ with $i + j \le k = 1$. The required index triples are $(0,0,1)$, $(0,1,1)$ and $(1,0,1)$.

$$\begin{aligned}&H(0,0,1) \overset{a_0}{=} \frac{\binom{n-1}{1}}{1}v(0)(\mathrm{i}\partial_t)^1_{t=\omega(0)\cdot l}a_0(t, x+l, -\omega(0))\\ &= (n-1)\mathrm{i}\partial_{t=|l|}a_0(t, x+l, -l/|l|) = (n-1)\mathrm{i}\partial_{t=|l|}\exp(A_{x+l+t(-\frac{l}{|l|})\frac{1}{2}}(t(-l/|l|))\\ &\overset{a_0}{=} (n-1)\mathrm{i}(A^{\mathrm{D}}_{-\frac{l}{|l|2}}(-l) + A_{x+l/2}(-l/|l|))\\ &\qquad = (n-1)\mathrm{i}(\frac{1}{2|l|}A^{\mathrm{D}}_l(l) - \frac{1}{2|l|}A^{\mathrm{D}}_l(l) - \frac{1}{|l|}A_x(l)) = -\frac{(n-1)\mathrm{i}}{|l|}A_x(l)\end{aligned}$$

Per definitionem H does not contain any exponential terms, see Section 4.4. Therefore, this calculation does not only show that

$$H(0,0,1) \overset{a_0}{=} -\frac{(n-1)\mathrm{i}}{|l|} A_x(l) \qquad \text{but also} \quad H(0,0,1) = -\frac{(n-1)\mathrm{i}}{|l|} A_x(l)\,.$$

For the calculation of $H(0,1,1)$ we additionally need some z-derivatives of v and ω. Those derivatives are given in Theorem A.6 but here we only need the following:

Remark 4.29. The first derivatives of ω have the following values at $z = 0$:

$$\omega(0) = \frac{l}{|l|}\,, \qquad \partial_{z_i=0}\omega = W_i\,, \qquad \partial^2_{z_i=0}\omega = -l/|l|\,,$$

where there is no summation over $i \in \{1,\dots,n-1\}$. Thus,

$$\Delta_{z=0}\omega = -(n-1)l/|l| \qquad \text{and} \qquad \partial_{z_i=0}\omega \cdot l = 0$$

The first derivatives of v have the following values at $z = 0$.

$$v(0) = 1\,, \qquad \partial_{z_i=0}v = 0\,, \qquad \partial^2_{z_i=0}v = -\frac{n-3}{4}$$

Again, there was no summation over the indices and therefore

$$\Delta_{z=0}v = \frac{3-n}{4} \cdot (n-1)\,.$$

In the calculation of wave invariants the term $K(z) \coloneqq \langle \omega(z), l\rangle \cdot \omega(z)$ will appear often. K has the following derivatives at $z = 0$.

$$K(0) = l\,, \qquad \partial_{z_i} K_{|z=0} = |l| W_i\,, \qquad \Delta_{z=0}K = -2l(n-1)\,.$$

With those z-derivatives we can compute $H(0,1,1)$. Eventually, we will compute the integral $\langle H(0,1,1), E_{-Fl}\rangle$ and for all constants C, not depending on x, $\langle C, E_{-Fl}\rangle = 0$. Thus, it is not necessary to compute additive constants and we simply denote these by C_i. Furthermore, we use that odd derivatives of v vanish at $z = 0$ and we sometimes abbreviate $K(z)$ by K.

$$\begin{aligned}
H(0,1,1) &\overset{a_0}{=} -\frac{1}{2\mathrm{i}|l|}\Delta_{z=0}v(z)a_0(\omega(z)l, x+l, -\omega(z)) \\
&= \frac{\mathrm{i}}{2|l|}\frac{3-n}{4}(n-1)a_0(|l|, x+l, -l/|l|) + \frac{\mathrm{i}}{2|l|}\Delta_{z=0}a_0(\omega(z)l, x+l, -\omega(z)) \\
&\overset{a_0}{=} C_1 + \frac{\mathrm{i}}{2|l|}\Delta_{z=0}\exp(A_{x+l-K(z)/2}(-K(z))) \\
&= C_1 + \frac{\mathrm{i}}{2|l|}\partial_{z_k=0}\exp(A_{x+l-K/2}(-K))(A^{\mathrm{D}}_{-\partial_{z_k}K/2}(-K) + A_{x+l-K/2}(-\partial_{z_k}K))
\end{aligned}$$

$$\begin{aligned}
&\overset{a_0}{=} C_1 + \frac{\mathrm{i}}{2|l|}\Big((A^{\mathrm{D}}_{\partial_{z_k}K/2}(K) + A_{x+l-K/2}(-\partial_{z_k}K))^2 \\
&\qquad + A^{\mathrm{D}}_{\Delta_z K/2}(K) + A^{\mathrm{D}}_{\partial_{z_k}K/2}(\partial_{z_k}K) - A_{x+l-K/2}(\Delta_z K)\Big)|_{z=0} \\
&= C_2 + \frac{\mathrm{i}}{2|l|}\Big((A^{\mathrm{D}}_{|l|W_k/2}(l) - A_{x+l/2}(|l|W_k))^2 - A^{\mathrm{D}}_x(-2l(n-1))\Big) \\
&= C_2 + \frac{\mathrm{i}}{2|l|}\Big(|l|^2(\frac{1}{2}(A^{\mathrm{D}}_{W_k}(l) - A^{\mathrm{D}}_l(W_k)) - A^{\mathrm{D}}_x(W_k) - \tilde{a}(W_k))^2 + 2(n-1)A^{\mathrm{D}}_x(l)\Big) \\
&= C_2 + \frac{\mathrm{i}}{2|l|}\Big(|l|^2(\frac{1}{2}\tilde{F}(l,W_k) - \tilde{a}(W_k) - A^{\mathrm{D}}_x(W_k))^2 + 2(n-1)A^{\mathrm{D}}_x(l)\Big) \\
&= C_3 + \frac{\mathrm{i}|l|}{2}A^{\mathrm{D}}_x(W_k)^2 - \mathrm{i}|l|A^{\mathrm{D}}_x(W_k)(\frac{1}{2}\tilde{F}(l,W_k) - \tilde{a}(W_k)) + \frac{\mathrm{i}(n-1)}{|l|}A^{\mathrm{D}}_x(l)
\end{aligned}$$

We have used Lemma 1.15 to introduce the curvature form $A^{\mathrm{D}}_X(Y) - A^{\mathrm{D}}_Y(X) = -\tilde{F}(X,Y)$. Similarly,

$$\begin{aligned}
&H(1,0,1) = \frac{\binom{n-2}{0}}{1}(\mathrm{i}\partial_{t=|l|})^0 a_1(t, x+l, -l/|l|) \overset{a_0}{=} \frac{\mathrm{i}}{2}|l|A_1(|l|, x+l, -l/|l|) \\
&= C_4 + \frac{\mathrm{i}|l|}{2}\cdot\Big(\frac{1}{|l|^2}A^{\mathrm{D}}_x(l)^2 + \frac{2}{|l|^2}\tilde{a}(l)A^{\mathrm{D}}_x(l) + A^{\mathrm{D}}_x\tilde{F}(l) - A^{\mathrm{D}^2}_x - 2\tilde{a}A^{\mathrm{D}}_x + Q(x+l\tau_1)\Big)
\end{aligned}$$

Adding those three terms we obtain

$$\begin{aligned}
&H(0,0,1) + H(0,1,1) + H(1,0,1) \cong \\
&C_5 + \frac{\mathrm{i}|l|}{2}\Big(A^{\mathrm{D}}_x(W_k)^2 - A^{\mathrm{D}}_x(W_k)(\tilde{F}(l,W_k) - 2\tilde{a}(W_k)) \\
&\quad + A^{\mathrm{D}}_x(l/|l|)^2 - A^{\mathrm{D}^2}_x + A^{\mathrm{D}}_x(l/|l|)2\tilde{a}(l/|l|) + A^{\mathrm{D}}_x(\tilde{F}(l) - 2\tilde{a}) + Q(x+l\tau_1)\Big),
\end{aligned}$$

where $\cong$ denotes a combination of the notations introduced so far. We can simplify this expression a bit further using Notation 4.25. If we replace the basis $\{W_1, \ldots, W_{n-1}, l/|l|\}$ in all traces by the standard basis we have for example $A^{\mathrm{D}}_x(W_k)^2 = A^{\mathrm{D}^2}_x - A^{\mathrm{D}}_x(l/|l|)^2$ and with $F(l,l) = 0$ those unwanted terms cancel:

$$\begin{aligned}
&C_5 + \frac{\mathrm{i}|l|}{2}\Big(A^{\mathrm{D}}_x(W_k)^2 - A^{\mathrm{D}}_x(W_k)(\tilde{F}(l,W_k) - 2\tilde{a}(W_k)) \\
&\quad + A^{\mathrm{D}}_x(l/|l|)^2 - A^{\mathrm{D}^2}_x + A^{\mathrm{D}}_x(l/|l|)2\tilde{a}(l/|l|) + A^{\mathrm{D}}_x(\tilde{F}(l) - 2\tilde{a}) + Q(x+l\tau_1)\Big) \\
&\qquad\qquad \overset{e_i}{=} C_5 + \frac{\mathrm{i}|l|}{2}Q(x+l\tau_1)
\end{aligned}$$

Hence, for $l \in \mathcal{L}\backslash\{0\}$ the first partial wave invariant is given by

$$\begin{aligned}
\mathsf{WI}_{1,l}(a,Q) &= \sum_{i+j\le 1}\langle H(i,j,1), E_{-Fl}\rangle = \langle C_5 + \frac{\mathrm{i}|l|}{2}Q(\,.\,+l\tau_1), E_{-Fl}\rangle \\
&= \frac{\mathrm{i}|l|}{2}\langle\sum_{c\in\mathcal{L}'}Q_cE_c\cdot E_c(l\tau_1), E_{-Fl}\rangle = \frac{\mathrm{i}|l|}{2}Q_{-Fl}E_{-Fl}(l\tau_1) \overset{\tau}{=} \frac{\mathrm{i}|l|}{2}Q_{-Fl},
\end{aligned}$$

where Q_c are the Fourier coefficients of Q with respect to the Hilbert basis $\{E_c\}_{c\in\mathcal{L}'}$ given in Theorem 2.3 and where we have used that $E_{-Fl}(l\tau_1) = \exp(\tilde{F}(l,l)\tau_1) = 1$. We have therefore proven the following statement.

Lemma 4.30. Given a flat torus M of even dimension with a nondegenerate Hermitian line bundle ω given by the curvature form $-\tilde{F}$. For all translation-invariant connections $a \in \mathbb{R}^{n'}$ the first wave invariant of $d \in |\mathcal{L}|\backslash\{0\}$,

$$\mathsf{WI}_{1,d}(a,Q) = \frac{\mathrm{i}|l|}{2}\sum_{|l|=d} E_a(l)\sigma_l Q_{-Fl}\,,$$

is a spectral invariant for every smooth potential $Q \in C^\infty(M)$.

Remark 4.31. Observe that in the final form the first partial wave invariant

$$\mathsf{WI}_{1,l}(a,Q) = \frac{\mathrm{i}|l|}{2}Q_{-Fl}$$

does not contain the 1-form a, it contains no terms of the form A_x^{D} and all terms that are free of Q vanish. We will show in the next section that those three conditions must, in fact, hold for all partial wave invariants. Using this we can introduce more notations that simplify the calculation of the second wave invariant to a manageable size.

We end this section with some remarks on the form in which this first wave invariant was given in [GGKW08] and why the results therein are true despite the sign error pointed out in Remark 4.19.

Lemma 4.30 is a generalization of [GGKW08, Corollary 4.2], which we reproduce in our notation:

Corollary 4.32 ([GGKW08, Corollary 4.2]).
If $\mathcal{L}$ is a nondegenerate lattice and for Chern invariant factors all equal to 1 then

$$E_a(Gc)Q_{-c} + E_a(-Gc)Q_c$$

is an invariant of $\mathrm{Spec}(a,Q)$ for every $c \in \mathcal{L}'\backslash\{0\}$. Recall that by Definition 2.5 $G := F^{-1}\colon \mathbb{R}^{n'} \to \mathbb{R}^n$.

Proof. Since all Chern invariant factors are 1, i.e. $r_i = 1$ for $i = 1,\dots,n/2$, we have that $Gc \in \mathcal{L}\backslash\{0\}$. As $\mathcal{L}$ is nondegenerate there are only two lattice vectors of length $|Gc|$, namely Gc and $-Gc$. Furthermore, $\sigma_{Gc} = \sigma_{-Gc}$, confer Definition 4.22. It follows that the first wave invariant of $|Gc| \in |\mathcal{L}|\backslash\{0\}$ is

$$\begin{aligned}\mathsf{WI}_{1,|Gc|}(a,Q) &= \frac{\mathrm{i}|Gc|}{2}\cdot\Big(E_a(Gc)\sigma_{Gc}Q_{-FGc} + E_a(-Gc)\sigma_{-Gc}Q_{FGc}\Big)\\ &= \frac{\mathrm{i}|Gc|}{2}\sigma_{Gc}\cdot\Big(E_a(Gc)Q_{-c} + E_a(-Gc)Q_c\Big)\end{aligned}$$

and the result follows because the factor $\frac{\mathrm{i}|Gc|}{2}\sigma_{Gc}$ depends only on fixed data.□

A variant of this corollary without the nondegeneracy assumption on $\mathcal{L}$ was used on [GGKW08, page 2474]. For more details see Theorem 6.32.

Remark 4.33. The formula that corresponds to our first partial wave invariant $\mathsf{WI}_{k,l}(a,Q)$ was computed in [GGKW08, Proposition C.6] to be (in our notation and up to integration over $\mathcal{F}$)

$$C_1(x,l) = g(x,l) + \frac{\mathrm{i}}{2}e_l(x)^{-1}a_0\Big(|l|, x+l, -\frac{l}{|l|}\Big)\int_0^{|l|} Q\Big(x-\tau\frac{l}{|l|}\Big)\,\mathrm{d}\tau\,,$$

where $g(x,l)$ is a function independent of Q. This is happens to be true despite the sign error described in Remark 4.19: By Lemma 4.23 the second summand equals

$$\frac{\mathrm{i}}{2}E_{Fl}(x)E_a(l)\sigma_l\cdot|l|\int_0^1 Q(x-\tau l)\,\mathrm{d}\tau$$

and integration over $\mathcal{F}$ yields

$$\operatorname{Vol} M\frac{\mathrm{i}}{2}E_a(l)\sigma_l|l|Q_{-Fl}\,,$$

which agrees with our first partial wave invariant (up to coefficients).

However, this $C_1(x,l)$ leads to spectral invariants (when integrated over x and summed over $|l|=d$) only if the function g vanishes. The sign error in [GGKW08] results in a nonvanishing function g, which is a violation of Necessary Condition 2 that will be given in Lemma 4.40. Furthermore, g is nonconstant with respect to the translation-invariant connection $\tilde{a}$, which is a violation of the Necessary Condition 1 of Lemma 4.37.

The authors of [GGKW08] continue by arguing that $\tilde{C}_1(x,l) \coloneqq \frac{2}{\mathrm{i}}(C_1(x,l) - g(x,l))$ is also a spectral invariant; thereby removing those terms that should have been zero in the first place. It follows that the sign error has no effect on the results obtained by using the first wave invariant as given in [GGKW08].

4.6 Necessary Conditions

In the previous section we have computed the first wave invariant and we have seen that the intermediate expressions have the form of polynomials in A^{D}, $\tilde{a}$ and Q. This, of course, holds for all wave invariants as can be easily seen from Section 4.4. On the other hand, we know negative spectral results resulting from the transplantations studied in Chapter 2. Those negative results must be reflected in all spectral invariants including the wave invariants.

The aim of this section is to find *necessary conditions* which the wave invariants must satisfy by being spectral invariants. Those conditions can than be used in two ways: We can remove certain terms from the calculation of the higher wave invariants, thereby simplifying the calculation. Alternatively we may choose not to utilize the necessary conditions for the (MATHEMATICA) computation and use the necessary conditions instead a posteriori as a heuristic mean to test for the correctness of the computations.

The necessary conditions also give general information about the wave invariants that allow us to obtain more general spectral information than the first five wave invariants. They also give some information about the limitations of information encoded in the wave invariants.

Let us first give a general form of the summands of the wave invariants: We assume that all 1-forms A_x have been replaced by $A_x^{\mathrm{D}} + \tilde{a}$ such that the partial wave invariants are given as polynomials depending on Q, A^{D} and $\tilde{a}$. We assume that all sums are in expanded form. The necessary conditions give restraints on the precise form of those polynomials.

Definition 4.34 (Multi-argument notation).
For any finite set $X = \{X_1 \ldots, X_k\}$ and a linear $\mathbb{C}$-valued map B we abbreviate

$$B(X) \coloneqq B(X_1) \cdots B(X_k).$$

If $X = \emptyset$ it is understood that the product is 1.

In the following we choose the coefficients C such that other parts of each summand, such as the dimension n or numerical factors like 2, i or $|l|$, are hidden within C but the appearances of A_x^{D} and $\tilde{a}$ are not.

The following proposition is clear from the definitions:

Proposition 4.35. The partial wave invariants are of the form

$$\mathsf{WI}_{k,l}(a, Q) = \sum_{s \in \mathcal{S}_k} \langle C_s(Q)(x) A_x^{\mathrm{D}}(X_s) \tilde{a}(Y_s), E_{-Fl}(x) \rangle_x \,,$$

where $\mathcal{S}_k$ is an index set for the summands in the expanded partial wave invariant and C is free of A_x^{D} and free of $\tilde{a}$. It is clear (but does not matter) that

$$X_s, Y_s \subset \{l, W_i, e_i\} \,.$$

The aim of this section is to show that the partial wave invariants are in fact of a simpler form: We obtain the same invariant $\mathsf{WI}_{k,l}(a, Q)$ if we only sum over the subset $\mathcal{S}'_k \subset \mathcal{S}_k$ for which $X_s = Y_s = \emptyset$ and $C_s(Q)$ contains the potential Q at least once.

In Chapter 2 transplantations were constructed and the existence of such spectrum-preserving operators must be reflected in the wave invariants. We

can use this in order to formulate necessary conditions that must be fulfilled by the wave invariants.

We first need a technical lemma.

Lemma 4.36. Let $d \in |\mathcal{L}|\backslash\{0\}$. If, given constants $p_l \in \mathbb{C}$,

$$\sum_{|l|=d} E_a(l)p_l = \text{const}$$

as a function of $a \in \mathbb{R}^{n'}$ then we already have

$$p_l = 0 \qquad \text{for all lattice vectors } l \in \mathcal{L} \text{ with } |l| = d.$$

Proof. If the function

$$f\colon \mathbb{R}^{n'} \cong \mathbb{R}^n \to \mathbb{C} \qquad \text{with} \qquad f(a) := \sum_{|l|=d} E_a(l)p_l$$

is constant with respect to $a \in \mathbb{R}^{n'}$ then $\operatorname{grad}_a f(a)$ must vanish. Thus, for any fixed $l_1 \in \mathcal{L}$ with $|l_1| = d$:

$$0 = \langle \operatorname{grad}_a f(a), l_1\rangle = -2\pi\mathrm{i} \sum_{|l|=d} E_a(l) \cdot \langle l, l_1\rangle \cdot p_l\,.$$

Applying the gradient $k \in \mathbb{N}$ times yields

$$0 = \sum_{|l|=d} E_a(l) \cdot \langle l, l_1\rangle^k \cdot p_l\,.$$

The scalar product $\langle l, l_1\rangle$ has maximal absolute value for $l = \pm l_1$ and for all other $l \in \mathcal{L}$ with $|l| = d$

$$|\langle l, l_1\rangle| < \langle l_1, l_1\rangle = d^2\,.$$

From this it follows that

$$\frac{1}{d^{2k}} \sum_{\substack{|l|=d \\ l\neq\pm l_1}} E_a(l)\langle l, l_1\rangle^k p_l \to 0 \qquad \text{for } k \to \infty$$

and this in turn implies that

$$\begin{aligned} 0 &= \lim_{k\to\infty} \frac{1}{d^{2k}}\Big(\sum_{|l|=d} E_a(l)\langle l, l_1\rangle^k p_l - \sum_{\substack{|l|=d \\ l\neq\pm l_1}} E_a(l)\langle l, l_1\rangle^k p_l\Big) \\ &= \lim_{k\to\infty} \frac{1}{d^{2k}}\Big(E_a(l_1)d^{2k}p_{l_1} + E_a(-l_1)(-1)^k d^{2k} p_{-l_1}\Big) \\ &= \lim_{k\to\infty}\Big(E_a(l_1)p_{l_1} + E_a(-l_1)(-1)^k p_{-l_1}\Big), \end{aligned}$$

which implies that

$$p_{l_1} = 0 \qquad \text{and} \qquad p_{-l_1} = 0\,. \qquad \square$$

Lemma 4.37 (Necessary Condition 1).
The partial wave invariants $\mathsf{WI}_{k,l}(a, Q)$ are constant in $a \in \mathbb{R}^{n'}$.

Proof. For all even-dimensional tori M with a nondegenerate line bundle ω, for all translation-invariant connections given by $a \in \mathbb{R}^{n'}$ and for all potentials Q the Schrödinger operators

$$\Delta_a^{\mathrm{D}} + Q \qquad \text{and} \qquad \Delta_{a+b}^{\mathrm{D}} + Q$$

are isospectral if $b \in \mathcal{L}'$ by Proposition 1.23 and Remark 1.37. From this the claim can be deduced as follows.

Per definitionem each wave invariant is of the form

$$\sum_{|l|=d} E_a(l) \cdot P_l(a)\,,$$

where the $P_l(a)$ are polynomials in a. Here, we can identify $\mathcal{L} \cong \mathbb{Z}^n$ and $\mathbb{R}^{n'} \cong \mathbb{R}^n$. The $P_l(a)$ are then polynomials over $\mathbb{R}^n$ with complex coefficients that depend on the data of the flat torus (in particular its dimension), Schrödinger operator (Chern factors r and potential Q) and the number of the wave invariant under consideration. The goal is to show that all those polynomials $P_l(a)$ are in fact constant with respect to a.

From the isospectrality of a and $a + b$ it follows that

$$\sum_{|l|=d} E_a(l) \cdot P_l(a) = \sum_{|l|=d} E_{a+b}(l) \cdot P_l(a+b) = \sum_{|l|=d} E_a(l) \cdot P_l(a+b)\,.$$

Further, we can write the polynomials $P_l(a)$ as a sum of homogeneous polynomials. Denote these homogeneous polynomials by $p_l^i(a)$ such that

$$P_l(a) = \sum_{i=0}^{K_l} p_l^i(a) \qquad \text{with} \qquad p_l^i(\lambda a) = \lambda^i p_l^i(a) \quad \text{for all } \lambda \in \mathbb{R}.$$

Let $K := \max_{|l|=d} K_l$. Then for all $z \in \mathbb{Z}\backslash\{0\}$ and all $b \in \mathcal{L}' \cong \mathbb{Z}^n$ we have on the one hand that

$$\begin{aligned}\frac{1}{z^K} \sum_{|l|=d} E_a(l) P_l(a+zb) &= \frac{1}{z^K} \sum_{|l|=d} E_a(l) \sum_{i=0}^{K_l} p_l^i(a+zb) \\ &= \sum_{|l|=d} E_a(l) \sum_{i=0}^{K_l} z^{i-K} p_l^i(a/z+b) \to \sum_{\substack{|l|=d \\ K_l=K}} E_a(l) p_l^K(b) \qquad \text{for } z \to \infty.\end{aligned}$$

On the other hand

$$\sum_{|l|=d} E_a(l) P_l(a + zb)$$

is constant as a sequence with respect to $z \in \mathbb{N}$. Therefore,

$$\frac{1}{z^K} \sum_{|l|=d} E_a(l) P_l(a + zb) \to 0 \qquad \text{for } z \to \infty$$

as long as $K > 0$. Comparing both limits implies

$$\sum_{|l|=d} E_a(l) p_l^K(b) = 0 \qquad \text{for all } a \in \mathbb{R}^{n'} \text{ and } b \in \mathcal{L}'.$$

Therefore, by Lemma 4.36

$$p_l^K(b) = 0 \qquad \text{for all } b \in \mathcal{L}' \cong \mathbb{Z}^n \text{ if } K > 0.$$

Thus, if $K > 0$ then p_l^K is a polynomial with zero set $\mathbb{Z}^n$ and must thus vanish: $p_l^K = 0$ for every $l \in \mathcal{L}$ with $|l| = d$.

In conclusion, the only nonvanishing homogeneous parts of $P_l(a)$ are $p_l^0(a)$, which are the constants with respect to a. □

Corollary 4.38. Because the partial wave invariants do not depend on a we can choose $a = 0$ for our calculations and we can write

$$\mathsf{WI}_{k,l}(Q) \coloneqq \mathsf{WI}_{k,l}(0, Q)\,.$$

Corollary 4.39. If all translation-invariant connections $a \in \mathbb{R}^{n'}$ are isospectral with respect to a given potential Q then all partial wave invariants must vanish,

$$\mathsf{WI}_{k,l}(Q) = 0 \qquad \text{for all } k \in \mathbb{N} \text{ and } l \in \mathcal{L}\backslash\{0\}.$$

Proof. By Lemma 4.37 all partial wave invariants are constant as a function of $a \in \mathbb{R}^{n'}$. If all translation-invariant connections are isospectral then the wave invariants

$$\mathsf{WI}_{k,d}(a, Q) = \sum_{|l|=d} E_a(l) \sigma_l \mathsf{WI}_{k,l}(Q) \qquad \text{with } d \in |\mathcal{L}|\backslash\{0\}$$

are also constant in a. Lemma 4.36 implies the corollary. □

The next lemma generalizes an observation already made in the case of $\mathsf{WI}_{1,l}(Q)$, see page 70.

Lemma 4.40 (Necessary Condition 2).
Let $k \in \mathbb{N}$ and $l \in \mathcal{L}\backslash\{0\}$. Those summands in the partial wave invariant $\mathsf{WI}_{k,l}(Q)$ that do not contain the potential Q cancel, more precisely

$$\mathsf{WI}_{k,l}(0) = 0\,.$$

Proof. Corollary 2.8 implies that for all flat tori and any connections given by $a \in \mathbb{R}^{n'}$ and $b \in \mathbb{R}^{n'}$ the two Schrödinger operators

$$\Delta_a^{\mathrm{D}} \qquad \text{and} \qquad \Delta_b^{\mathrm{D}}$$

are isospectral. Thus, if the potential vanishes then all wave invariants

$$\sum_{|l|=d} E_a(l) \cdot P_l(Q)$$

are constant as a function of $a \in \mathbb{R}^{n'}$. By Lemma 4.37 the $P_l(Q)$ are independent of a and Lemma 4.36 implies

$$P_l(Q) = 0 \qquad \text{if } Q = 0.$$

The statement follows from $P_l(Q) = \mathsf{WI}_{k,l}(Q)\sigma_l$. □

Finally, we show that the partial wave equations that contain A_x^{D} must cancel. Using that the partial wave invariants are independent of a we have the following lemma.

Lemma 4.41 (Necessary Condition 3).
If $\mathcal{S}'_k \subset \mathcal{S}_k$ is the subset with $X_s \neq \emptyset$ (and $Y_s = \emptyset$) then

$$\sum_{s\in\mathcal{S}'_k} \langle C_s(Q)(x) A_x^{\mathrm{D}}(X_s), E_{-Fl}(x)\rangle_x = 0$$

in the notation of Proposition 4.35.

Proof. Note first that X_s is always independent of x, there is no $A_x^{\mathrm{D}}(x)$ within the wave invariants and $A_x^{\mathrm{D}}(X_s)$ is always $|X_s|$-linear in x. By writing out the x-integral the left hand side is equal to

$$\frac{1}{\operatorname{Vol} M} \int_{\mathcal{F}} \sum_{s\in\mathcal{S}'_k} C_s(Q)(x) A_x^{\mathrm{D}}(X_s) E_{Fl}(x)\,\mathrm{d}x$$

for any choice fundamental domain $\mathcal{F}$ of the lattice $\mathcal{L}$. Both $C_s(Q)(x)$ and $E_{Fl}(x)$ are $\mathcal{L}$-periodic in x and therefore

$$\frac{1}{\operatorname{Vol} M} \int_{\mathcal{F}} \sum_{s\in\mathcal{S}'_k} C_s(Q)(x) A_{x+h}^{\mathrm{D}}(X_s) E_{Fl}(x)\,\mathrm{d}x$$

must be constant with respect to $h \in \mathcal{L}$.

As in the proof of Lemma 4.37 it now follows (via replacing h by zh, $z \in \mathbb{N}$, and considering degrees of homogeneity in h) that those summands with $X_s \neq \emptyset$ cancel. □

The following theorem combines the necessary conditions of the previous lemmata.

Theorem 4.42. The partial wave invariants do not depend on a and are free of A_x^{D}. Each summand must contain the potential Q. If $\mathcal{S}'_k \subset \mathcal{S}_k$ is the subset of such summands then

$$\mathsf{WI}_{k,l}(Q) = \sum_{s \in S'_k} \langle C_s(Q), E_{-Fl} \rangle .$$

4.7 The Second Wave Invariant

We use the necessary conditions of Section 4.6 to introduce some more notations that will shorten the computations of the second wave invariant to a more manageable size.

Notation 4.43 (Necessary Conditions).
We write $A \overset{\mathrm{NC}}{=} B$ if A and B differ by terms that must vanish by the necessary conditions of Section 4.6, i.e. if $A - B$ consists of terms containing A_x^{D}, $\tilde{a}$ or that are free of Q.

Of course, $A \overset{\mathrm{NC}}{=} B$ does not imply $Q \cdot A \overset{\mathrm{NC}}{=} Q \cdot B$ nor $\Box(a_0 tA) \overset{\mathrm{NC}}{=} \Box(a_0 tB)$ and we have to be careful only to use this abbreviation after all occurrences of Q have been taken into account and after all derivatives have been computed.

Notation 4.44. We write $A \overset{x}{=} B$ if $\langle A, E_{-Fl} \rangle = \langle B, E_{-Fl} \rangle$, where it is assumed that l is an arbitrary but fixed nonzero lattice vector. Additionally, we want to apply this abbreviation only to parts of sums. Thus, we also write

$$A + C \overset{x}{=} B + C \qquad \text{if } A \overset{x}{=} B.$$

Again, we write $A \cong B$ if A and B are equal up to a combination of the abbreviations "$\overset{\mathrm{NC}}{=}$", "$\overset{x}{=}$" or "$\overset{a_0}{=}$".

If $\quad H(i,j,k) \cong H_{i,j,k} \quad$ then

$$\mathsf{WI}_{k,l}(Q) = \sum_{i+j \leq k} \langle H(i,j,k), E_{-Fl} \rangle = \sum_{i+j \leq k} \langle H_{i,j,k}, E_{-Fl} \rangle .$$

Further, the fact that there are no A_x^{D}-terms and thus no x-dependence other than via the potentials Q allows us to x-integrate terms that are linear in Q.

Definition 4.45. Given a smooth function Q on $\mathbb{R}^n$ and a finite set of vectors $d = \{d_1, \dots, d_h\} \subset \mathbb{R}^n$ we denote by

$$Q(x,d) \coloneqq \partial_{i_1} \cdots \partial_{i_h} Q(x) (d_1)_{i_1} \cdots (d_h)_{i_h}$$

the multiple derivative of Q in the direction of the vectors given by d.

Definition 4.46. By abuse of notation we write

$$Q_{-Fl}(x) \coloneqq Q_{-Fl} E_{-Fl}(x)\,.$$

For those coefficients C that are free of Q and hence do not depend on x we have $\langle CQ(x+\tau l), E_{-Fl}\rangle = CQ_{-Fl}$, because $E_{Fl}(x) = E_{Fl}(x+\tau l)$ since $Fl(\tau l) = 0$. In particular, $Q(x+\tau l) \overset{x}{=} Q(x)$. In this case, we can evaluate the τ-integrals without further assumptions about the potential Q. For example,

$$\tau_2 Q(x+\tau_1\tau_2 l) \overset{x}{=} \tau_2 Q(x) \overset{x}{=} \tau_2 Q_{-Fl}(x) \overset{\tau}{=} \frac{1}{2} Q_{-Fl}(x)\,.$$

Additionally, if we have derivatives of Q given by some set d then

$$Q(x+\tau l, d) \overset{x}{=} Q(x,d) \overset{x}{=} Q_{-Fl} E_{-Fl}(x,d) = Q_{-Fl} \cdot \tilde{Fl}(d)$$

with the multi-argument notation of Definition 4.34. In particular, if $l \in d$ then $Q(x+\tau l, d) \overset{x}{=} 0$ and the corresponding integrals vanish.

4.7.1 Calculations

The calculation of the second wave invariant is similar to the calculation of the first wave invariant but involves more triples (i,j,k) with $i+j \le k$ for which H must be evaluated: $(0,0,2)$, $(1,0,2)$, $(2,0,2)$, $(0,1,2)$, $(1,1,2)$ and $(0,2,2)$.

Recalling the recipe from Section 4.4, let us start with the trivial computations. The symbol a_0 does not depend on the potential Q and therefore

$$H(0,0,2) \overset{a_0}{=} \frac{\binom{n-1-0}{2-0-0}}{1} v(0) (\mathrm{i}\partial)^{2-0-0}_{t=\omega(0)l} a_0(t, x+l, -\omega(z)) \overset{\mathrm{NC}}{=} 0$$

Analogously,

$$H(0,1,2) \overset{\mathrm{NC}}{=} 0 \overset{\mathrm{NC}}{=} H(0,2,2)\,.$$

In order to compute those triples (i,j,k) with $i=1$ or $i=2$ we need a_1 and a_2, respectively. Already, a_1 has a rather lengthy expression, see page 67, and a_2 would be even longer. Luckily we do actually not need to compute the whole of a_2.

Definition 4.47. If we compute a_i as prescribed by the recipe of Section 4.4 and write the result in expanded form we obtain a uniquely determined expression describing a_i. With this expression we have a well-defined decomposition of a_i as $a_i = a_i^Q + a_i^{\neg Q}$, where a_i^Q is the part of a_i containing the potential and $a_i^{\neg Q}$ is the part free of the potential. Alternatively, $a_i^{\neg Q}$ is obtained by setting Q to zero in a_i and $a_i^Q := a_i - a_i^{\neg Q}$.

With this notation

$$a_1^Q(t,x,\omega) = a_0 \frac{\mathrm{i}}{2} t Q(x + (1-\tau_1)t\omega)$$

and thus, with $v(0) = 0$ and $\omega(0) = l/|l|$,

$$\begin{aligned}
H(1,0,2) &\overset{a_0}{=} \frac{\binom{n-1-1}{2-0-1}}{1} v(0)(\mathrm{i}\partial_t)^{2-1}_{t=\omega(0)l} a_1(t, x+l, -\omega(0)) \\
&\overset{\text{NC}}{=} (n-2)\mathrm{i}\partial_{t=|l|} a_1^Q(t, x+l, -l/|l|) \\
&= (n-2)\mathrm{i}\partial_{t=|l|}\Big(a_0(t, x+l, -l/|l|)\frac{\mathrm{i}}{2} t Q(x + l - (1-\tau_1)tl/|l|)\Big) \\
&\overset{\text{NC}}{=} \frac{2-n}{2}\Big(Q(x+\tau_1 l) - Q(x+\tau_1 l, \{l\})(1-\tau_1)\Big) \\
&\overset{x}{=} \frac{2-n}{2}\Big(Q_{-Fl}(x) + Q_{-Fl}(x)\tilde{Fl}(l)(1-\tau_1)\Big) \\
&= \frac{2-n}{2} Q_{-Fl}(x)
\end{aligned}$$

For the computation of $H(1,1,2)$ we need the z-derivatives of ω, v and K given in Theorem A.6. Recall that $K(z) = \langle \omega(z), l\rangle \omega(z)$. There are no further x-derivatives to compute in $H(1,1,2)$ beyond those already evaluated for a_1^Q. Thus, by the necessary conditions we can use

$$a_0(\omega(z)l, x+l, -\omega(z)) = \exp(A_{x+l-K/2}(-K)) \overset{\text{NC}}{=} \exp(A^{\mathrm{D}}_{K/2-l}(K))$$

to obtain

$$\begin{aligned}
H(1,1,2) &\cong \frac{\binom{n-1-1}{2-1-1}}{1(-2\mathrm{i}|l|)^1} \Delta_{z=0} v(z)(\mathrm{i}\partial_t)^{2-1-1}_{t=\omega(z)l} a_1^Q(t, x+l, -\omega(z)) \\
&\overset{\text{NC}}{=} \frac{\mathrm{i}}{2|l|}\Delta_{z=0} v(z) \exp(A^{\mathrm{D}}_{K/2-l}(K))\frac{\mathrm{i}}{2}\omega(z) l Q(x + l - (1-\tau_1)K(z))\,.
\end{aligned}$$

Because single ∂_{z_i}-derivatives of v and ωl vanish at $z = 0$ we have a "Leibniz rule" for the z-Laplacian. Also, $\Delta_{z=0}\omega l = -(n-1)|l|$, $\Delta_{z=0} v = -1/4(n-1)(n-3)$ and $K(0) = l$.

$$
\begin{aligned}
H(1,1,2) \cong -\frac{1}{4|l|}\Big(&\Delta_{z=0} v(z)|l| \cdot Q(x+\tau_1 l) \\
&+ \Delta_{z=0}\omega(z) l\, Q(x+\tau_1 l) \\
&+ |l|\Delta_{z=0} \exp(A^{\mathrm{D}}_{K/2-l}(K)) \cdot Q(x+l-(1-\tau_1)K)\Big) \\
\overset{x}{=} \frac{1}{16}(n-1)(n-3)Q_{-Fl}(x) &+ \frac{1}{4}(n-1)Q_{-Fl}(x) \\
&+ \frac{-1}{4}\partial_{z_k=0} a_0 \cdot (A^{\mathrm{D}}_{\partial_{z_k}K/2}(K) + A^{\mathrm{D}}_{K/2-l}(\partial_{z_k}K))\cdot \\
&\qquad Q(x+l-(1-\tau_1)K) \\
&- \frac{1}{4}\partial_{z_k=0} a_0 Q(x+l-(1-\tau_1)K, \{\partial_{z_k}K\})(\tau_1-1)
\end{aligned}
$$

We therefore have, where the right hand side is to be evaluated at $z=0$, that

$$
\begin{aligned}
H(1,1,2) \cong \frac{n^2-1}{16}&Q_{-Fl}(x) \\
&- \frac{1}{4}(A^{\mathrm{D}}_{\partial_{z_k}K/2}(K) + A^{\mathrm{D}}_{K/2-l}(\partial_{z_k}K))^2 Q_{-Fl}(x) \\
&- \frac{1}{4}(A^{\mathrm{D}}_{\Delta_z K/2}(K) + 2A^{\mathrm{D}}_{\partial_{z_k}K/2}(\partial_{z_k}K) + A^{\mathrm{D}}_{K/2-l}(\Delta_z K))Q_{-Fl}(x) \\
&- \frac{1}{2}(A^{\mathrm{D}}_{\partial_{z_k}K/2}(K) + A^{\mathrm{D}}_{K/2-l}(\partial_{z_k}K)) \\
&\qquad Q(x+l-(1-\tau_1)K, \{\partial_{z_k}K\})(\tau_1-1) \\
&- \frac{1}{4}Q(x+l-(1-\tau_1)K, \{\partial_{z_k}K, \partial_{z_k}K\})(\tau_1-1)^2 \\
&- \frac{1}{4}Q(x+l-(1-\tau_1)K, \{\Delta_{z_k}K\})(\tau_1-1)\,.
\end{aligned}
$$

Additionally, we can integrate terms containing derivatives of Q and use $\partial_{z_k=0}K = |l|W_k$ and $\Delta_{z=0}K = -2l(n-1)$.

$$
\begin{aligned}
H(1,1,2) \cong -\frac{1}{4}Q_{-Fl}(x)\Big(&\frac{1-n^2}{4} + (A^{\mathrm{D}}_{|l|W_k/2}(l) - A^{\mathrm{D}}_{l/2}(|l|W_k))^2 \\
&+ (A^{\mathrm{D}}_{-2l(n-1)/2}(l) + 2A^{\mathrm{D}}_{|l|W_k/2}(|l|W_k) - A^{\mathrm{D}}_{l/2}(-2l(n-1))) \\
&+ 2(A^{\mathrm{D}}_{|l|W_k/2}(l) - A^{\mathrm{D}}_{l/2}(|l|W_k))\tilde{F}l(|l|W_k)(\tau_1-1) \\
&+ \tilde{F}l(|l|W_k)^2(\tau_1-1)^2\Big)
\end{aligned}
$$

Evaluating the τ-integrals and replacing $A^{\mathrm{D}}_{W_k}(l) - A^{\mathrm{D}}_{l}(W_k)$ by $\tilde{F}(l, W_k)$ yields

$$
H(1,1,2) \cong -\frac{1}{4}Q_{-Fl}(x)\Big(\frac{1-n^2}{4} + \frac{|l|^2}{12}\tilde{F}(l,W_k)^2 + |l|^2 A^{\mathrm{D}}_{W_k}(W_k)\Big)
$$

It remains to calculate H for the last triple: $(2,0,2)$. Here, we would need a_2 but thanks to the necessary condition of Lemma 4.40 a_2^Q is sufficient.

$$H(2,0,2) \cong \frac{\binom{n-1-2}{2-0-2}}{1} v(0)(\mathrm{i}\partial_t)^0_{t=\omega(0)\cdot l} a_2^Q(t, x+l, -\omega(0)) \\ \overset{a_0}{=} \frac{\mathrm{i}}{2}|l| A_2^Q(|l|, x+l, -l/|l|)$$

Hence, we need (only) A_2^Q and this can be computed more efficiently by applying the wave operator selectively to a_1. We use

$$\left(Q a_1^{\neg Q} + \Box a_1^Q\right)/a_0 \to_2 A_2^Q .$$

As no differential operators are applied to A_2^Q we can directly use the final arguments on the right hand side of "$\to_2$". We replace

$$(t, x, \omega) \qquad \text{by} \\ (|l|\tau_2, x + l - (1-\tau_2)|l| l/|l|, -l/|l|) = (|l|\tau_2, x + \tau_2 l, -l/|l|) ,$$

use the necessary conditions and denote both steps by "$\rightsquigarrow$". For example,

$$Q\frac{\mathrm{i}}{2} t A_x^{\mathrm{D}}(\omega)^2 \rightsquigarrow Q(x+\tau_2 l)\frac{\mathrm{i}}{2}|l|\tau_2 A^{\mathrm{D}}_{x+\tau_2 l}(-l/|l|)^2 \overset{\mathrm{NC}}{=} Q(x+\tau_2 l)\frac{\mathrm{i}\tau_2}{2|l|} A^{\mathrm{D}}_{\tau_2 l}(l)^2 \\ \overset{x}{=} \frac{\mathrm{i}\tau_2^3}{2|l|} Q_{-Fl}(x) A_l^{\mathrm{D}}(l)^2 \overset{\tau}{=} \frac{\mathrm{i}}{8|l|} Q_{-Fl}(x) A_l^{\mathrm{D}}(l)^2 .$$

Applying the same transformation to all terms of A_1 given on page 67,

$$\begin{aligned} A_1^{\neg Q} \overset{\mathrm{NC}}{=} & A_x^{\mathrm{D}}(\omega)^2 + 2t A_x^{\mathrm{D}}(\omega) A_\omega^{\mathrm{D}}(\omega) + t^2 A_\omega^{\mathrm{D}}(\omega)^2 + A_\omega^{\mathrm{D}}(\omega) - \frac{1}{3} t^2 A^{\mathrm{D}}(\omega)^2 \\ & - A^{\mathrm{D}} - A_x^{\mathrm{D}} A^{\mathrm{D}}(\omega) t - \frac{1}{3} A_\omega^{\mathrm{D}} A^{\mathrm{D}}(\omega) t^2 - A_x^{\mathrm{D}^2} - t A_x^{\mathrm{D}} A_\omega^{\mathrm{D}} - \frac{1}{3} A_\omega^{\mathrm{D}^2} t^2 \\ A_1^Q = & Q(x + (1-\tau_1) t\omega) , \end{aligned}$$

yields

$$Q\frac{\mathrm{i}}{2} t A_1^{\neg Q} \rightsquigarrow \frac{\mathrm{i}}{2} Q_{-Fl}(x)\Big(\\ \frac{1}{2|l|} A_l^{\mathrm{D}}(l) - \frac{|l|}{12} A_l^{\mathrm{D}^2} + \frac{|l|}{6} A_l^{\mathrm{D}} A^{\mathrm{D}}(l) - \frac{|l|}{12} A^{\mathrm{D}}(l)^2 - \frac{|l|}{2} A^{\mathrm{D}}\Big).$$

The wave operator consists of six terms

$$\Box = \partial_t^2 - \partial_{x_i}^2 - A^{\mathrm{D}}_{e_i}(e_i) - 2A_x(e_i)\partial_{x_i} - A_x(e_i)^2 + Q(x)$$

that we apply separately to a_1^Q, in order of increasing complexity:

$$
\begin{aligned}
&-A^{\mathrm{D}} a_0 \frac{\mathrm{i}}{2} tQ(x+(1-\tau_1)t\omega) \rightsquigarrow -A^{\mathrm{D}} \frac{\mathrm{i}}{2}|l|\tau_2 Q_{-Fl}(x) \overset{\tau}{=} -A^{\mathrm{D}} \frac{\mathrm{i}}{4}|l| Q_{-Fl}(x)\\
&-A_x^2 a_1^Q \rightsquigarrow -A^{\mathrm{D}}_{\tau_2 l}{}^2 \frac{\mathrm{i}}{2}|l|\tau_2 Q_{-Fl}(x) \overset{\tau}{=} -A^{\mathrm{D}2}_{l} \frac{\mathrm{i}}{8}|l| Q_{-Fl}(x)\\
&-2A_x(e_i)\partial_{x_i} a_1^Q \underset{\mathrm{NC}}{\overset{a_0}{=}} -A_x(e_i)\mathrm{i}\Big(A^{\mathrm{D}}_{e_i}(t\omega) t A_1^Q + tQ(x+(1-\tau_1)t\omega, \{e_i\})\Big)\\
&\qquad \rightsquigarrow -A^{\mathrm{D}}_{\tau_2 l}\mathrm{i}\Big(A^{\mathrm{D}}(-\tau_2 l)|l|\tau_2 Q_{-Fl}(x) + |l|\tau_2 Q_{-Fl}(x)\tilde{F}l\Big)\\
&\qquad \overset{\tau}{=} \Big(\frac{1}{4}A^{\mathrm{D}}_l A^{\mathrm{D}}(l) - \frac{1}{3}A^{\mathrm{D}}_l \tilde{F}l\Big)\mathrm{i}|l| Q_{-Fl}(x)
\end{aligned}
$$

The double derivatives are rather lengthy. Details of the following two calculations are left to the reader. We abbreviate $\chi := x + (1-\tau_1)t\omega$ and $\xi := x + \tau_1\tau_2 l$. Then,

$$
\begin{aligned}
-\partial_{x_i}^2 a_1^Q &\overset{a_0}{=} -\frac{\mathrm{i}}{2}t^3 A^{\mathrm{D}}_{e_i}(\omega)^2 Q(\chi) - \mathrm{i}t^2 A^{\mathrm{D}}_{e_i}(\omega) Q(\chi, \{e_i\}) - \frac{\mathrm{i}}{2} tQ(\chi, \{e_i, e_i\})\\
&\rightsquigarrow -\frac{\mathrm{i}}{2}|l|\tau_2^3 A^{\mathrm{D}}_{e_i}(l)^2 Q(\xi) + \mathrm{i}|l|\tau_2^2 A^{\mathrm{D}}_{e_i}(l) Q(\xi, \{e_i\}) - \frac{\mathrm{i}}{2}|l|\tau_2 Q(\xi, \{e_i, e_i\})\\
&\cong -\mathrm{i}|l| Q_{-Fl}(x)\Big(\frac{1}{8}A^{\mathrm{D}}(l)^2 - \frac{1}{3}A^{\mathrm{D}}(l)\tilde{F}l + \frac{1}{4}\tilde{F}l^2\Big).
\end{aligned}
$$

It is not difficult to see that in the following summand all derivatives of Q vanish. If we subsume corresponding terms into $D(Q)$ we have:

$$
\begin{aligned}
\partial_t^2 a_1^Q &= (\partial_t^2 a_0)\frac{\mathrm{i}}{2} tQ(\chi) + (\partial_t a_0)\mathrm{i}Q(\chi) + D(Q)\\
&\rightsquigarrow \Big(\Big(A^{\mathrm{D}}_{\tau_2 l}(-l/|l|) + |l|\tau_2 A^{\mathrm{D}}_{-l/|l|}(-l/|l|)\Big)^2 + \frac{1}{|l|^2}A^{\mathrm{D}}_l(l)\Big)\frac{\mathrm{i}}{2}|l|\tau_2 Q(\xi)\\
&\quad + \Big(A^{\mathrm{D}}_{\tau_2 l}(-l/|l|) + |l|\tau_2 A^{\mathrm{D}}_{-l/|l|}(-l/|l|)\Big)\mathrm{i}Q(\xi)\\
&\cong \frac{\mathrm{i}}{4|l|}A^{\mathrm{D}}_l(l) Q_{-Fl}(x)\,.
\end{aligned}
$$

The last term of the wave operator is different from all other terms, because it gives a term quadratic in Q. In particular, we cannot x-integrate the term as easily as the other terms.

$$
Qa_0\frac{\mathrm{i}}{2}tA_1^Q \rightsquigarrow \frac{\mathrm{i}}{2}|l|\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l)
$$

Adding all terms (including the ones from $Qa_1^{\neg Q}$ and the general factor

$\mathrm{i}|l|/2$ from the definition of $a_2(|l|, x+l, -l/|l|)$), gives $H(2,0,2)$.

$$\begin{aligned}
H(2,0,2) \cong & -\frac{|l|}{4}Q_{-Fl}(x)\Big(\frac{1}{2|l|}A_l^{\mathrm{D}}(l) - \frac{|l|}{12}A_l^{\mathrm{D}^2} + \frac{|l|}{6}A_l^{\mathrm{D}}A^{\mathrm{D}}(l) - \frac{|l|}{12}A^{\mathrm{D}}(l)^2 \\
& - \frac{|l|}{2}A^{\mathrm{D}} - A^{\mathrm{D}}\frac{|l|}{2} - A_l^{\mathrm{D}^2}\frac{|l|}{4} + \frac{|l|}{2}A_l^{\mathrm{D}}A^{\mathrm{D}}(l) - \frac{2|l|}{3}A_l^{\mathrm{D}}\tilde{F}l \\
& - \frac{|l|}{4}A^{\mathrm{D}}(l)^2 + \frac{2|l|}{3}A^{\mathrm{D}}(l)\tilde{F}l - \frac{|l|}{2}\tilde{F}l^2 + \frac{1}{2|l|}A_l^{\mathrm{D}}(l)\Big) \\
& - \frac{1}{4}|l|^2\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l)
\end{aligned}$$

Collecting summands and $\tilde{F}l = A^{\mathrm{D}}(l) - A_l^{\mathrm{D}}$ yields

$$\begin{aligned}
H(2,0,2) \cong & -\frac{|l|}{4}Q_{-Fl}(x)\Big(\frac{1}{|l|}A_l^{\mathrm{D}}(l) - |l|A^{\mathrm{D}} \\
& - \frac{|l|}{3}A_l^{\mathrm{D}^2} + \frac{2|l|}{3}A_l^{\mathrm{D}}A^{\mathrm{D}}(l) - \frac{|l|}{3}A^{\mathrm{D}}(l)^2 + \frac{|l|}{6}\tilde{F}l^2\Big) \\
& - \frac{1}{4}|l|^2\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l) \\
= & -\frac{|l|}{4}Q_{-Fl}(x)\Big(\frac{1}{|l|}A_l^{\mathrm{D}}(l) - |l|A^{\mathrm{D}} - \frac{|l|}{6}\tilde{F}l^2\Big) \\
& - \frac{1}{4}|l|^2\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l)\,.
\end{aligned}$$

This result for $H(2,0,2)$ is rather short considering that a_2 consists of 696 summands.

We can now add all $H(i,j,2)$ with $i+j \le 2$ to obtain the second wave invariant.

Lemma 4.48 (Second Wave Invariant).
For all $d \in |\mathcal{L}|\backslash\{0\}$, all translation-invariant connections $a \in \mathbb{R}^{n'}$ and all potentials $Q \in C^\infty(M)$ the second wave invariant is

$$\mathsf{WI}_{2,d}(a,Q) = \sum_{|l|=d} E_a(l)\sigma_l \cdot \mathsf{WI}_{2,l}(Q) \qquad \text{with the partial wave invariant}$$

$$\mathsf{WI}_{2,l}(Q) = \Big(\frac{n_{3,5}}{16} + \frac{|l|^2}{48}\tilde{F}(l)^2\Big)\cdot Q_{-Fl} - \frac{|l|^2}{8}\sum_{\substack{c_1\in\mathcal{L}'\\ c_1(l)=0}} Q_{c_1}Q_{-c_1-Fl}\,.$$

Here, $n_{3,5} \coloneqq (n-3)(n-5)$.

Proof. Consider

$$\begin{aligned}
H &\coloneqq H(0,0,2)+H(0,1,2)+H(0,2,2)+H(1,0,2)+H(1,1,2)+H(2,0,2)\\
&\cong 0+0+0+\frac{2-n}{2}Q_{-Fl(x)}\\
&\quad-\frac{1}{4}Q_{-Fl}(x)\Big(\frac{1-n^2}{4}+\frac{|l|^2}{12}\tilde{F}(l,W_k)^2+|l|^2A^{\mathrm{D}}_{W_k}(W_k)\Big)\\
&\quad-\frac{|l|}{4}Q_{-Fl}(x)\Big(\frac{1}{|l|}A^{\mathrm{D}}_l(l)-|l|A^{\mathrm{D}}-\frac{|l|}{6}\tilde{F}l^2\Big)\\
&\quad-\frac{1}{4}|l|^2\tau_2Q(x+\tau_2l)Q(x+\tau_1\tau_2l)
\end{aligned}$$

Changing the basis of the traces from $\{W_k, l/|l|\}$ to $\{e_i\}$ gives

$$\begin{aligned}
H &\cong Q_{-Fl}(x)\Big(\frac{n_{3,5}}{16}-\frac{|l|^2}{48}\tilde{F}(l)^2-\frac{|l|^2}{4}A^{\mathrm{D}}+\frac{|l|^2}{4}A^{\mathrm{D}}_{l/|l|}(l/|l|)\\
&\qquad\qquad-\frac{1}{4}A^{\mathrm{D}}_l(l)+\frac{|l|^2}{4}A^{\mathrm{D}}+\frac{|l|^2}{24}\tilde{F}l^2\Big)\\
&\qquad\qquad-\frac{1}{4}|l|^2\tau_2Q(x+\tau_2l)Q(x+\tau_1\tau_2l)\\
&= Q_{-Fl}(x)\Big(\frac{n_{3,5}}{16}-\frac{|l|^2}{48}\tilde{F}l^2+\frac{|l|^2}{24}\tilde{F}l^2\Big)\\
&\qquad\qquad-\frac{1}{4}|l|^2\tau_2Q(x+\tau_2l)Q(x+\tau_1\tau_2l)\,.
\end{aligned}$$

The second partial wave invariant is defined as

$$\mathsf{WI}_{2,l}(Q)=\langle H,E_{-Fl}\rangle\,.$$

The τ-integration performed in Example B.9,

$$\tau_2Q(x+\tau_2l)Q(x+\tau_1\tau_2l)\overset{x}{=}\sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1(l)=0=c_2(l)}}Q_{c_1}Q_{c_2}E_{c_1+c_2}(x)\frac{1}{2}\,,$$

implies the claim. □

Remark 4.49. While the first wave invariant was given in [GGKW08] the second wave invariant was computed only partially and only under very narrow assumptions. The result that is closest to our formulation of the wave invariants is [GGKW08, Theorem C.9]: For a nondegenerate lattice $\mathcal{L}$ and $a=0$ the second wave invariant for $l\in|\mathcal{L}|\backslash\{0\}$ is given by (in their notation)

$$\begin{aligned}
C_{2,l}=-\frac{1}{4}\int_{\mathcal{F}}e^{-2\pi\mathrm{i}e_l(x)}a_0\Big(|l|,x+l,-\frac{l}{|l|}\Big)\cdot\Big(\int_0^{|l|}Q^-(x-\tau l/|l|)\,\mathrm{d}\tau\Big)^2\,\mathrm{d}x\\
+\text{ terms which do not involve } Q^-\,.
\end{aligned}$$

The even and odd parts Q^+ and Q^- are defined in Definition 6.30.

This happens to be true despite the sign error in [GGKW08] described in Remark 4.19. We first rewrite $C_{2,l}$. By Lemma 4.23 the term $e^{-2\pi i e_l(x)} a_0(|l|, x + l, -l/|l|)$ translates to $E_{Fl}(x)\sigma_l$ in our notation. Thus,

$$C_{2,l} = -\frac{\sigma_l |l|^2}{4} \operatorname{Vol} M \cdot \langle \Big(\int_0^1 Q^-(x - \tau l)\, \mathrm{d}\tau \Big)^2, E_{-Fl} \rangle \\ + \text{terms which do not involve } Q^- .$$

On the other hand, we can rewrite our second wave invariant for nondegenerate lattices and $a = 0$ as follows: Let $\alpha := \frac{n_{3,5}}{16} + \frac{|l|^2}{48}\tilde{F}(l)^2$ and $d = |l| = |-l| \in |\mathcal{L}|\backslash\{0\}$.

$$\begin{aligned}
\sigma_l \mathsf{WI}_{2,d}(0, Q) &= \sigma_l^2 \cdot \mathsf{WI}_{2,l}(Q) + \sigma_{-l}\sigma_l \cdot \mathsf{WI}_{2,-l}(Q) \\
&= \alpha(Q_{-Fl} + Q_{Fl}) - \frac{|l|^2}{8} \Big(\sum_{\substack{c_1 + c_2 = -Fl \\ c_1(l) = c_2(l) = 0}} Q_{c_1} Q_{c_2} + \sum_{\substack{c_1 + c_2 = Fl \\ c_1(-l) = c_2(-l) = 0}} Q_{c_1} Q_{c_2} \Big) \\
&= 2\alpha \langle Q^+, E_{-Fl} \rangle - \frac{|l|^2}{8} \langle \Big(\int_0^1 Q(\,.\, - l\tau)\, \mathrm{d}\tau \Big)^2, E_{Fl} + E_{-Fl} \rangle \\
&= 2\alpha \langle Q^+, E_{-Fl} \rangle - \frac{|l|^2}{8} \langle \Big(\int_0^1 Q^+(\,.\, - l\tau)\, \mathrm{d}\tau \Big)^2, E_{Fl} + E_{-Fl} \rangle \\
&\qquad - \frac{|l|^2}{8} \langle \Big(\int_0^1 Q^-(\,.\, - l\tau)\, \mathrm{d}\tau \Big)^2, E_{Fl} + E_{-Fl} \rangle .
\end{aligned}$$

In the last step we have used $Q = Q^+ + Q^-$ and the fact that the integrals of the mixed term $2Q^+Q^-$ vanish, because $2Q^+Q^-$ is an odd function while $E_{Fl} + E_{-Fl}$ is even.

It follows that $C_{2,l}$ in the vague form given in [GGKW08, Theorem C.9] agrees with our second wave invariant (up to our choice of normalization by $\operatorname{Vol} M$) and the statement of [GGKW08, Theorem C.9] is true.

However, if one computes the second wave invariant with the sign error described in Remark 4.19 it turns out that the term of second order in Q is unaffected while the lower order terms do change. In particular, the resulting formula is in violation of the necessary conditions of Lemma 4.40 and Lemma 4.41. One can also compute $C_{2,l}$ without assuming that $a = 0$. Then $C_{2,l}$ is also in violation of the necessary condition of Lemma 4.37. It follows that $C_{2,l}$ of [GGKW08] is in fact not a spectral invariant if computed completely.

4.7.2 Outlook on higher wave invariants

The calculation of higher wave invariants could, in principle, be done in much the same way. We have to distinguish different cases with respect to the dimension n, though, and the τ-integration becomes more difficult. However, the complexity of the necessary calculations increases very rapidly and there are no obvious, additional simplifications that would reduce the number of summands appearing in the $H(i,j,k)$ with $k > 2$ in the same way as the notations did in the case $k = 2$.

The following table shows the number of summands appearing in the calculation of the k-th wave invariant. The first column gives the wave invariant in question, the second the number of triples (i,j,k) with $i + j \leq k$ for each k and the third column gives the number of summands within $\sum_{i+j\leq k} H(i,j,k)$. The latter value depends of course on the way this sum is expressed and on what simplifications are (not) applied. Here all summands that are free of Q or contain $\tilde{a}$ are dropped. However, no further x- or τ-integration is performed and the sum is expanded. Additionally, we assume that the dimension n is *"large"*, $n > k-1$, for each wave invariant.

The last column gives the number of summands within the small partial wave invariants as given in Theorem 5.8.

k	$\#(i,j,k)$	Summands in $\sum H(i,j,k)$	Summands in $\mathsf{wi}_{k,l}(Q)$
1	3	1	1
2	6	48	2
3	10	1 984	4
4	15	78 545	10
5	21	3 210 748	92

It seems clear that the manual calculation of higher invariants is not feasible (and for that reasons none were given in [GGKW08]). On the other hand, despite the very large intermediate expressions the wave invariants can be simplified to a reasonable size. Both the computation and the simplifications can be computed using the MATHEMATICA notebook given in Appendix D and in digital form in [Ber18].

Chapter 5

Higher Wave Invariants

5.1 Wave Invariants

To express the wave invariants more explicitly several definitions and notations are required. Those will be introduced in the following.

The τ-integration within the calculation of the wave invariants gives different results depending on whether sums of various $c_i(l)$ with $c_i \in \mathcal{L}'$ vanish or not. Also, the wave invariants contain only terms with $c_i \in \mathcal{L}'$ such that $\sum c_i = -Fl$. To express the τ-integrals we will use the concept of *cases* and Q-sums over those *cases*.

The definition of the *cases* requires some use of *formal* notation. If we write, say, $\mathfrak{c}_i \equiv \sum \pm c_j$ in the following definition, then this means that $\mathfrak{c}_i$ is a formula given by the string of symbols on the right hand side of this equivalence.

Definition 5.1 (Case).
For $l \in \mathcal{L}\backslash\{0\}$ a *case* is a subset

$$l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q] \subset (\mathcal{L}')^q \,,$$

where in the place of $\mathfrak{c}_i$ we can either have 0 or c_i or some sum $\sum \pm c_j$ with $j < i$. A tuple $c \in (\mathcal{L}')^q$ is in $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$ if and only if the following holds:

- If $\mathfrak{c}_i \equiv 0$, then $c_i(l) = 0$.
- If $\mathfrak{c}_i \equiv c_i$, then for all $1 \leq s \leq i$ the following sum is nonvanishing $c_s(l) + \cdots + c_i(l) \neq 0$.
- If $\mathfrak{c}_i \equiv \sum \pm c_j$, then $c_i(l) = \sum \pm c_j(l)$.

Additionally, $c_1 + \cdots + c_k = -Fl$ must hold.

Example 5.2. Let $l \in \mathcal{L}\backslash\{0\}$. Then,

(1) $l[0,0] = \{(c_1, c_2) \in \mathcal{L}' \times \mathcal{L}' \mid c_1(l) = c_2(l) = 0 \text{ and } c_2 = -c_1 - Fl\}$

(2) $l[c_1, -c_1] = \{(c_1, c_2) \in \mathcal{L}' \times \mathcal{L}' \mid 0 \neq c_1(l) = -c_2(l) \text{ and } c_2 = -c_1 - Fl\}$

(3) $l[c_1, c_2, -c_1 - c_2]$ is the set consisting of $(c_1, c_2, c_3) \in \mathcal{L}' \times \mathcal{L}' \times \mathcal{L}'$ such that $c_1(l) \neq 0$, $c_2(l) \neq 0$, $c_1(l) + c_2(l) \neq 0$, $c_3(l) = -c_1(l) - c_2(l)$ and $c_3 = -c_1 - c_2 - Fl$.

(4) $l[0, c_2, -c_2, c_2, -c_2]$ is the set consisting of $(c_1, c_2, c_3, c_4, c_5)$ such that $c_1(l) = 0$, $c_2(l) \neq 0$, $c_3(l) = -c_2(l)$, $c_4(l) = c_2(l)$, $c_5(l) = -c_2(l)$ and $c_5 = -c_1 - c_2 - c_3 - c_4 - Fl$.

Since $Fl(l) = 0$ the cases in the examples are all consistent. A case of the form $l[c_1, c_2]$, however, is an empty set.

Definition 5.3 (Traces).
Given some $c \in \mathcal{L}'^q$ and $1 \leq i, j \leq q$ we define

$$\tilde{c}_{i,j} \coloneqq \operatorname{Tr}(\tilde{c}_i \tilde{c}_j) = \sum_{h=1}^{n} \tilde{c}_i(e_h)\tilde{c}_j(e_h)$$

and for such a c we also write

$$\operatorname{Tr} \tilde{c}^2 \coloneqq \tilde{c}_{1,1} + \cdots + \tilde{c}_{q,q} \,.$$

Additionally, for $k \in \mathbb{N}$ it is understood that

$$\tilde{c}_{i,j}^k \coloneqq (\tilde{c}_{i,j})^k = \left(\operatorname{Tr}(\tilde{c}_i \tilde{c}_j)\right)^k \qquad \text{and} \qquad \operatorname{Tr}^k \tilde{c}^2 \coloneqq (\operatorname{Tr} \tilde{c}^2)^k \,.$$

We extend the *curvature traces* $\tilde{F}_k$ of Definition 3.7 to $c_i, c_j \in \mathcal{L}'$. We write

$$\tilde{F}_k(\tilde{c}_i, \tilde{c}_j) \coloneqq \sum_{h_1, h_2 = 1}^{n} \tilde{c}_i(e_{h_1}) \tilde{F}_k(e_{h_1}, e_{h_2}) \tilde{c}_j(e_{h_2}) \,.$$

Recall that there are k factors $2\pi\mathrm{i}$ within the curvature traces $\tilde{F}_k$ and $k+2$ such factors in $\tilde{F}_k(\tilde{c}_i, \tilde{c}_j)$.

Definition 5.4. For any $n \in \mathbb{N}$ and two odd $i < j \in \mathbb{Z}$ let

$$n_{i,j} \coloneqq \prod_{i \leq k \leq j \text{ odd}} (n - k) \,.$$

For example, $n_{3,5} = (n-3)(n-5)$.

Definition 5.5 (Q-sum).
For some subset $C \subset (\mathcal{L}')^q$ and some $f \colon C \to \mathbb{C}$ the corresponding Q-sum is defined to be

$$\sum_{c \in C}^{Q} f(c) \coloneqq \sum_{c \in C} Q_c \cdot f(c) \,,$$

where $Q_c = Q_{c_1} \cdots Q_{c_q}$ is the product of the Fourier coefficients of the potential Q with respect to the dual lattice vectors $c = (c_1, \ldots, c_q)$.

Theorem 5.6 (Explicit Wave Invariants).
For a flat torus M of even dimension n with a nondegenerate Hermitian line bundle ω such that the curvature form of a translation-invariant connection $a \in \mathbb{R}^{n'}$ is $-\tilde{F}$ and a smooth, real-valued potential Q on M the first wave invariants

$$\mathsf{WI}_{k,d}(a,Q) = \sum_{|l|=d} E_a(l)\sigma_l \mathsf{WI}_{k,l}(Q) \qquad \text{with } d \in |\mathcal{L}|\backslash\{0\}$$

are given by

$$\begin{aligned}
\mathsf{WI}_{1,l}(Q) &= \frac{i|l|}{2} Q_{-Fl} \\
\mathsf{WI}_{2,l}(Q) &= Q_{-Fl}\Big(\frac{n_{3,5}}{16} - \frac{|l|^2}{48}\tilde{F}_2(l,l)\Big) - \sum_{c\in l[0,0]}^{Q} \frac{|l|^2}{8} \\
\mathsf{WI}_{3,l}(Q) &= Q_{-Fl}\Big(\mathrm{i}|l|^3(\frac{\tilde{F}_2}{96} - \frac{\tilde{F}_2(l,l)^2}{2304}) - \frac{n_{1,7}}{256|l|}\mathrm{i} + \frac{\mathrm{i}|l|n_{5,7}}{384}\tilde{F}_2(l,l)\Big) \\
&\quad + \sum_{c\in l[0,0]}^{Q}\Big(\frac{\mathrm{i}}{192}|l|^3 \operatorname{Tr}\tilde{c}^2 + \frac{n_{5,7}\mathrm{i}}{64}|l|\Big) - \sum_{c\in l[c_1,-c_1]}^{Q} \frac{\mathrm{i}|l|^3\tilde{c}_{1,2}}{8\tilde{c}_1(l)^2} - \sum_{c\in l[0,0,0]}^{Q} \frac{\mathrm{i}|l|^3}{48} \\
\mathsf{WI}_{4,l}(Q) &= Q_{-Fl}\cdot\Big(-|l|^4(\frac{\tilde{F}_2\tilde{F}_2(l,l)}{2304} - \frac{\tilde{F}_2(l,l)^3}{165888} + \frac{\tilde{F}_4(l,l)}{2880}) - \frac{n_{-1,9}}{6144|l|^2} \\
&\qquad + \frac{n_{3,9}}{6144}\tilde{F}_2(l,l) + |l|^2(\frac{n_{7,9}}{768}\tilde{F}_2 - \frac{n_{7,9}}{18432}\tilde{F}_2(l,l)^2)\Big) \\
&\quad + \sum_{c\in l[0,0]}^{Q}\Big(\frac{n_{3,9}}{1024} + \frac{|l|^2 n_{7,9}}{1536}\operatorname{Tr}\tilde{c}^2 + \frac{|l|^4}{46080}(5\operatorname{Tr}^2\tilde{c}^2 - 120\tilde{F}_2 + 4\tilde{c}_{1,2}^2)\Big) \\
&\quad + \sum_{c\in l[c_1,-c_1]}^{Q} \frac{-|l|^4}{192\tilde{c}_1(l)^4}\Big(72\tilde{c}_{1,2}^2 - 24\tilde{c}_1(l)\tilde{F}_1(\tilde{c}_1,\tilde{c}_2) \\
&\qquad + \tilde{c}_1(l)^2\tilde{c}_{1,2}\cdot(\operatorname{Tr}(\tilde{c}_1+\tilde{c}_2)^2 + 3n_{7,9}/|l|^2)\Big) \\
&\quad + \sum_{c\in l[0,0,0]}^{Q}\Big(-\frac{|l|^4\operatorname{Tr}\tilde{c}^2}{1152} - \frac{|l|^2 n_{7,9}}{384}\Big) + \sum_{c\in l[0,c_2,-c_2]}^{Q} \frac{|l|^4\tilde{c}_{2,3}}{16\tilde{c}_2(l)^2} \\
&\quad + \sum_{c\in l[0,0,0,0]}^{Q} \frac{|l|^4}{384}
\end{aligned}$$

Proof. $\mathsf{WI}_{1,l}(Q)$ and $\mathsf{WI}_{2,l}(Q)$ were computed already in Chapter 4. The remaining wave invariants given in this Theorem are computed using the MATHEMATICA notebook given in Appendix D, where the first two are also computed again. In the fourth partial wave invariant we additionally use that

$$\tilde{c}_{1,1} + 2\tilde{c}_{1,2} + \tilde{c}_{2,2} = \operatorname{Tr}(\tilde{c}_1+\tilde{c}_2)^2\,. \qquad \square$$

The fifth wave invariant can also be obtained using this MATHEMATICA notebook. It has been omitted, for now, because of its length. We can remove

trivial factors and combine the different invariants to obtain simpler invariants, which we shall call "small" wave invariants. We again write those invariants as

$$\mathsf{wi}_{k,d}(a,Q) = \sum_{|l|=d} E_a(l)\sigma_l \cdot \mathsf{wi}_{k,l}(Q)\,,$$

where the $\mathsf{wi}_{k,l}(Q)$ are appropriately chosen linear combinations of the partial wave invariants $\mathsf{WI}_{k,l}(Q)$ given in Theorem 5.6 above. Note, however, that any coefficients used in those linear combinations may only depend on d but not on the lattice vectors l with $|l| = d$.

For the fifth small wave invariant we need one further multiindex notation.

Definition 5.7. For any $l \in \mathcal{L}\backslash\{0\}$ and $c \in \mathcal{L}'^q$ we write $\tilde{c}(l) = (\tilde{c}_1(l), \dots, \tilde{c}_q(l))$ and for $\alpha \in \mathbb{Z}^q$ we set

$$\tilde{c}(l)^\alpha := \tilde{c}_1(l)^{\alpha_1} \cdots \tilde{c}_q(l)^{\alpha_q}\,;$$

assuming that $\tilde{c}_i(l) > 0$ or $\alpha_i \geq 0$ for all $i \in \{1, \dots, q)$.

Thanks to the heat invariants, the following Theorem will actually hold for all $d \in |\mathcal{L}|$ including $d = 0$.

Theorem 5.8. Fix a flat torus M of even dimension n with a nondegenerate Hermitian line bundle ω such that the curvature form of the translation-invariant connections is $-\tilde{F}$. For a translation-invariant connection $a \in \mathbb{R}^{n'}$ and a smooth real-valued potential Q on M the *small wave invariants*

$$\mathsf{wi}_{k,d}(a,Q) = \sum_{|l|=d} E_a(l)\sigma_l \cdot \mathsf{wi}_{k,l}(Q)$$

given below are spectral invariants for all $d \in |\mathcal{L}|$.

$$\mathsf{wi}_{1,l}(Q) = Q_{-Fl}$$

$$\mathsf{wi}_{2,l}(Q) = Q_{-Fl}\frac{|\tilde{F}l|^2}{6} + \sum_{c\in l[0,0]}^{Q} 1$$

$$\mathsf{wi}_{3,l}(Q) = Q_{-Fl}\frac{|\tilde{F}l|^4}{48} - \sum_{c\in l[0,0]}^{Q}\frac{\operatorname{Tr}\tilde{c}^2}{4} + \sum_{c\in l[c_1,-c_1]}^{Q}\frac{6\tilde{c}_{1,2}}{\tilde{c}_1(l)^2} + \sum_{c\in l[0,0,0]}^{Q} 1$$

$$\begin{aligned}\mathsf{wi}_{4,l}(Q) = {} & Q_{-Fl}\Big(\frac{|\tilde{F}l|^6}{432} - \frac{2\tilde{F}_4(l,l)}{15}\Big) + \sum_{c\in l[0,0]}^{Q}\Big(\frac{\operatorname{Tr}^2\tilde{c}^2}{24} + \frac{\tilde{c}_{1,2}^2}{30}\Big)\\ & + \sum_{c\in l[c_1,-c_1]}^{Q}\frac{2}{\tilde{c}_1(l)^2}\Big(\frac{24\tilde{F}_1(\tilde{c}_1,\tilde{c}_2)}{\tilde{c}_1(l)} - \frac{72\tilde{c}_{1,2}^2}{\tilde{c}_1(l)^2} - \tilde{c}_{1,2}\operatorname{Tr}(\tilde{c}_1+\tilde{c}_2)^2\Big)\\ & - \sum_{c\in l[0,0,0]}^{Q}\frac{\operatorname{Tr}\tilde{c}^2}{3} + \sum_{c\in l[0,c_2,-c_2]}^{Q}\frac{24\tilde{c}_{2,3}}{\tilde{c}_2(l)^2} + \sum_{c\in l[0,0,0,0]}^{Q} 1\end{aligned}$$

$$
\begin{aligned}
\mathsf{wi}_{5,l}(Q) = \frac{Q_{-Fl}}{18}|\tilde{F}l|^2\Big(\frac{5}{1152}|\tilde{F}l|^6 - \tilde{F}_4(l,l)\Big)\\
+ \sum_{c\in I[0,0]}^{Q} \frac{1}{6048}\Big(-35(\operatorname{Tr}\tilde{c}^2)^3 + 4032\tilde{F}_2(\tilde{c}_1,\tilde{c}_1) - 84\operatorname{Tr}\tilde{c}^2\tilde{c}_{1,2}^2 - 16\tilde{c}_{1,2}^3\Big)\\
+ \sum_{c\in I[c_1,-c_1]}^{Q} \frac{5}{6\tilde{c}_1(l)^6}\Big(-5760\tilde{c}_1(l)\tilde{F}_1(\tilde{c}_1,\tilde{c}_2)\tilde{c}_{1,2} + 8640\tilde{c}_{1,2}^3\\
\qquad -48\tilde{c}_1(l)^3\tilde{F}_1(\tilde{c}_1,\tilde{c}_2)(\tilde{c}_{1,1}+3\tilde{c}_{1,2})\\
\qquad +144\tilde{c}_1(l)^2\Big(4\tilde{F}_2(\tilde{c}_1,\tilde{c}_2) + \tilde{c}_{1,2}^2(\tilde{c}_{1,1}+2\tilde{c}_{1,2})\Big)\\
\qquad +\tilde{c}_1(l)^4\tilde{c}_{1,2}\Big(\tilde{c}_{1,1}^2 + 2\tilde{c}_{1,2}^2 + \tilde{c}_{1,1}(4\tilde{c}_{1,2}+\tilde{c}_{2,2})\Big)\Big)\\
+ \sum_{c\in I[0,0,0]}^{Q} \frac{1}{6}\Big(\frac{5}{12}(\operatorname{Tr}\tilde{c}^2)^2 + \tilde{c}_{1,2}^2\Big)\\
+ \sum_{c\in I[0,c_2,-c_2]}^{Q} \frac{-10}{\tilde{c}_2(l)^4}\Big(-24\tilde{c}_2(l)\tilde{F}_1(\tilde{c}_2,\tilde{c}_3) - 24\tilde{c}_{1,2}\tilde{c}_{1,3} + 72\tilde{c}_{2,3}^2\\
\qquad +\tilde{c}_2(l)^2\tilde{c}_{2,3}\Big(\tilde{c}_{1,1}+2\tilde{c}_{2,2}+2\tilde{c}_{2,3}\Big)\Big)\\
+ \sum_{c\in I[c_1,c_2,-c_1-c_2]}^{Q} \frac{160\tilde{c}_{1,2}\tilde{c}_{1,3}}{\tilde{c}(l)^{(1,2,2)}}\Big(2\tilde{c}_1(l)+\tilde{c}_2(l)\Big)\\
+ \sum_{c\in I[0,0,0,0]}^{Q} -\frac{5}{12}\operatorname{Tr}\tilde{c}^2 + \sum_{c\in I[0,0,c_3,-c_3]}^{Q} \frac{60}{\tilde{c}_3(l)^2}\tilde{c}_{3,4} + \sum_{c\in I[c_1,-c_1,c_1,-c_1]}^{Q} \frac{-240}{\tilde{c}_1(l)^4}\Big(4\tilde{c}_{1,2}+\tilde{c}_{1,3}\Big)\\
+ \sum_{c\in I[c_1,c_2,-c_2,-c_1]}^{Q} \frac{240}{\tilde{c}_1(l)\tilde{c}_2(l)^3(\tilde{c}_1+\tilde{c}_2)(l)^2}\cdot\Big(\tilde{c}_1(l)^2(2\tilde{c}_{1,2}+\tilde{c}_{1,3}+3\tilde{c}_{2,3}+\tilde{c}_{2,4})\\
\qquad +\tilde{c}_1(l)\tilde{c}_2(l)(2\tilde{c}_{1,2}+2\tilde{c}_{1,3}+5\tilde{c}_{2,3}+2\tilde{c}_{2,4})\\
\qquad +\tilde{c}_2(l)^2(\tilde{c}_{1,3}+\tilde{c}_{1,4})\Big)\\
+ \sum_{c\in I[c_1,c_2,c_3,-c_1-c_2-c_3]}^{Q} \frac{60}{(\tilde{c}_1(l)+\tilde{c}_2(l))^2(\tilde{c}_2(l)+\tilde{c}_3(l))^2\tilde{c}(l)^{(2,2,2,2)}}\Big(\\
\qquad -2\tilde{c}(l)^{(6,1,1,0)}\Big(11\tilde{c}_{1,2}+10\tilde{c}_{2,3}+14\tilde{c}_{2,4}\Big)\\
\qquad +\tilde{c}(l)^{(5,3,0,0)}\Big(8\tilde{c}_{1,2}+8\tilde{c}_{1,3}-32\tilde{c}_{1,4}+6\tilde{c}_{2,3}-48\tilde{c}_{2,4}-40\tilde{c}_{3,4}\Big)\\
\qquad +\tilde{c}(l)^{(6,2,0,0)}\Big(-12\tilde{c}_{1,2}-6\tilde{c}_{1,3}-30\tilde{c}_{1,4}-5\tilde{c}_{2,3}-42\tilde{c}_{2,4}-25\tilde{c}_{3,4}\Big)\\
\qquad +\tilde{c}(l)^{(4,4,0,0)}\Big(6\tilde{c}_{1,2}+66\tilde{c}_{1,3}+28\tilde{c}_{1,4}-33\tilde{c}_{2,3}-78\tilde{c}_{2,4}-17\tilde{c}_{3,4}\Big)\\
\qquad +\tilde{c}(l)^{(5,2,1,0)}\Big(34\tilde{c}_{1,2}-8\tilde{c}_{1,3}-28\tilde{c}_{1,4}+42\tilde{c}_{2,3}+32\tilde{c}_{2,4}-14\tilde{c}_{3,4}\Big)\\
\qquad +2\tilde{c}(l)^{(4,3,1,0)}\Big(29\tilde{c}_{1,2}+28\tilde{c}_{1,3}+8\tilde{c}_{1,4}+17\tilde{c}_{2,3}+8\tilde{c}_{2,4}-\tilde{c}_{3,4}\Big)\\
\qquad -2\tilde{c}(l)^{(7,1,0,0)}\Big(7\tilde{c}_{1,2}+\tilde{c}_{1,4}+6\tilde{c}_{2,3}+10\tilde{c}_{2,4}+\tilde{c}_{3,4}\Big)\\
\qquad +4\tilde{c}(l)^{(3,3,2,0)}\Big(5\tilde{c}_{1,2}+20\tilde{c}_{1,3}+9\tilde{c}_{1,4}+\tilde{c}_{2,3}-6\tilde{c}_{2,4}+6\tilde{c}_{3,4}\Big)\\
\qquad +\tilde{c}(l)^{(4,2,2,0)}\Big(50\tilde{c}_{1,2}-2\tilde{c}_{1,3}-2\tilde{c}_{1,4}+57\tilde{c}_{2,3}+78\tilde{c}_{2,4}+9\tilde{c}_{3,4}\Big)\Big)\\
+ \sum_{c\in I[0,0,0,0,0]}^{Q} 1
\end{aligned}
$$

Proof. The first invariant is simply given by $\mathsf{wi}_{1,l} \coloneqq \mathsf{WI}_{1,l} \cdot 2/\mathrm{i}|l|$ or, equivalently, by $\mathsf{wi}_{1,d} \coloneqq \mathsf{WI}_{1,d} \cdot 2/\mathrm{i}|l|$. Both definitions are equivalent because the coefficient $2/\mathrm{i}|l|$ depends only on d but not on the lattice vectors l with $|l| = d$. The second small wave invariant is given by $\mathsf{wi}_{2,l} \coloneqq -(\mathsf{WI}_{2,l} - \mathsf{wi}_{1,l} \cdot n_{3,5}/16) \cdot 8/|l|^2$. Further $\tilde{F}_2(l,l) = \sum \tilde{F}(l,e_i)\tilde{F}(e_i,l) = -\operatorname{Tr} \tilde{F}l^2 = |\tilde{F}l|^2$.

Now, set

$$\mathsf{wi}_{3,l} \coloneqq (\mathsf{WI}_{3,l}/\mathrm{i} - \mathsf{wi}_{2,l}|l|n_{5,7}/64 + \mathsf{wi}_{1,l}(n_{1,7}/256|l| - \tilde{F}_2|l|^3/96)) \cdot (-48)/|l|^3 .$$

Notice that we consider $\tilde{F}$ and thus $\tilde{F}_2$ as fixed. Also, no coefficient depends on the choice of lattice vector $|l| = d$ and thus $\mathsf{wi}_{3,d}$ is well-defined. For the same reason, we may define

$$\begin{aligned}\mathsf{wi}_{4,l} \coloneqq \Big(\mathsf{WI}_{4,l} + \mathsf{wi}_{3,l}\frac{|l|^2 n_{7,9}}{384} + \mathsf{wi}_{2,l}\Big(-\frac{n_{3,9}}{1024} + \frac{120|l|^4}{46080}\tilde{F}_2\Big) \\ + \mathsf{wi}_{1,l}\Big(\frac{n_{-1,9}}{6144|l|^2} - |l|^2\frac{\tilde{F}_2 n_{7,9}}{768}\Big)\Big) \cdot \frac{384}{|l|^4} .\end{aligned}$$

The computation of the small wave invariants can also be found in the Mathematica notebook of Appendix D. For the fifth small wave invariant we additionally use some manual simplifications that can be found in Appendix D.2.

Note, however, that Theorem 5.6, which we use to construct the small wave invariants, only holds for $d \neq 0$. We can use the heat invariants given in Theorem 3.28 to show that the small wave invariants are indeed spectral invariants if $d = 0$.

In this case there is only one lattice vector $l = 0$ of length d and additionally $E_a(0) = \sigma_0 = 1$. Thus, the partial and nonpartial wave invariants agree. For the first wave invariant we have

$$\mathsf{wi}_{1,0}(a,Q) = \mathsf{wi}_{1,0}(Q) = Q_0 = -\mathsf{hi}_2(Q) = \frac{1}{\operatorname{Vol} M}\int_M Q(x)\,\mathrm{d}x$$

and thus $\mathsf{wi}_{1,0}$ is a spectral invariant.

We have $l[0,0] = 0[0,0] = \big\{c \in \mathcal{L}'^2 \mid c_i(0) = 0 \text{ and } c_1 + c_2 = -F0 = 0\big\} = \{(c,-c) \mid c \in \mathcal{L}'\}$. Thus, recalling that Q is real-valued and hence $\overline{Q_c} = Q_{-c}$:

$$\mathsf{wi}_{2,0}(Q) = 0 + \sum_{c\in\mathcal{L}'} Q_c Q_{-c} = \|Q\|^2_{\mathrm{L}^2} = 2\mathsf{hi}_4(Q) + \frac{\tilde{F}_2}{6} .$$

Again, since $\tilde{F}$ is fixed, $\mathsf{wi}_{2,0}(Q)$ is a spectral invariant.

More generally, all cases that are not of the form $l[0,\dots,0]$ must be empty sets as there can be no $c \in \mathcal{L}'$ with $c(0) \neq 0$. The Q-sums over cases that are of the form $l[0,\dots,0]$ are all integrals similar to the following:

$$\frac{1}{\operatorname{Vol} M}\int_M Q(x)^3\,\mathrm{d}x = \sum_{\substack{c_1,c_2,c_3\in\mathcal{L}'\\ c_1+c_2+c_3=0}} Q_{c_1}Q_{c_2}Q_{c_3} = \sum_{c\in 0[0,0,0]}^{Q} 1$$

and

$$\begin{aligned}\frac{1}{\operatorname{Vol} M}\int_M Q(x)\Delta Q(x)\,\mathrm{d}x &= \frac{1}{\operatorname{Vol} M}\int_M \sum_{c_1,c_2\in\mathcal{L}'} Q_{c_1}E_{c_1}(x)\cdot Q_{c_2}E_{c_2}(x)\tilde{c}_{2,2}\,\mathrm{d}x\\ &= \sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1+c_2=0}} Q_{c_1}Q_{c_2}\frac{\tilde{c}_{1,1}+\tilde{c}_{2,2}}{2} = \sum_{c\in 0[0,0]}^{Q}\frac{\operatorname{Tr}\tilde{c}^2}{2}\,.\end{aligned}$$

With the help of the MATHEMATICA notebook of Appendix D (or by a tedious calculation) we can show that

$$\begin{aligned}\mathsf{wi}_{3,0}(Q) &= -6\,\mathsf{hi}_6(Q) - \frac{\tilde{F}_2}{2}\mathsf{hi}_2(Q)\\ \mathsf{wi}_{4,0}(Q) &= 24\,\mathsf{hi}_8(Q) + 2\tilde{F}_2\mathsf{hi}_4(Q) + \frac{\tilde{F}_2^2}{12} - \frac{\tilde{F}_4}{15}\\ \mathsf{wi}_{5,0}(Q) &= -120\,\mathsf{hi}_{10}(Q) - 10\tilde{F}_2\mathsf{hi}_6(Q) - \Big(\frac{5}{12}\tilde{F}_2^2 - \frac{1}{3}\tilde{F}_4\Big)\mathsf{hi}_2(Q)\,.\end{aligned}$$

Thus, all five small wave invariants are spectral invariants even for $l = 0$. □

Now let again $d \neq 0$.

Lemma 5.9. For every $l \in \mathcal{L}$ with $|l| = d \neq 0$ there is at least one other lattice vector of the same length, $|-l| = d$. If $\mathcal{L}_{d+} \subset \mathcal{L}$ is a maximal set containing lattice vectors of length d but such that $l \in \mathcal{L}_{d+}$ implies $-l \notin \mathcal{L}_{d+}$ then

$$\mathsf{wi}_{k,d} = \sum_{l\in\mathcal{L}_{d+}} \sigma_l\cdot 2\operatorname{Re}\Big(E_a(l)\mathsf{wi}_{k,l}\Big) \qquad \text{for } k = 1,\dots,5.$$

The invariants are independent of the choice of $\mathcal{L}_{d+}$. If $\mathcal{L}$ is nondegenerate, then $\#\mathcal{L}_{d+} = 1$ and the sums over $l \in \mathcal{L}_{d+}$ consist of only one summand.

Proof. $\displaystyle \mathsf{wi}_{k,d} = \sum_{|l|=d}\sigma_l\cdot E_a(l)\mathsf{wi}_{k,l} = \sum_{l\in\mathcal{L}_{d+}}\Big(\sigma_l\cdot E_a(l)\mathsf{wi}_{k,l} + \sigma_{-l}\cdot E_a(-l)\mathsf{wi}_{k,-l}\Big)$

We have that $\sigma_{-l} = \sigma_l$ and $E_a(-l) = \overline{E_a(l)}$. If we knew additionally that $\mathsf{wi}_{k,-l} = \overline{\mathsf{wi}_{k,l}}$ then

$$\sigma_l\cdot E_a(l)\mathsf{wi}_{k,l} + \sigma_{-l}\cdot E_a(-l)\mathsf{wi}_{k,-l} = \sigma_l\cdot 2\operatorname{Re}(E_a(l)\mathsf{wi}_{k,l})$$

and the claim would follow.

We consider the partial wave invariants of Theorem 5.8 with respect to the lattice vector $-l$. Because Q is real-valued we have $\overline{Q_{-Fl}} = Q_{Fl}$ and thus the first partial wave invariant for $-l$ is $\mathsf{wi}_{1,-l} = Q_{-F(-l)} = Q_{Fl} = \overline{Q_{-Fl}} = \overline{\mathsf{wi}_{1,l}}$.

The coefficients of the Q_{-Fl}-terms in the partial wave invariants 2 to 5 are real and l appears in even order and hence those terms transform analogously. For the terms containing Q-sums over cases notice that if $c \in l[\mathfrak{c}_1, \dots, \mathfrak{c}_k]$ then $-c \in (-l)[\mathfrak{c}_1, \dots, \mathfrak{c}_k]$. Additionally, $\tilde{c}_i{}^2$ is real-valued and, thus, for example

$$\alpha_{-l} \coloneqq \sum_{c\in(-l)[0,0]}^{Q} \frac{\operatorname{Tr}\tilde{c}^2}{4} = \sum_{c\in l[0,0]} Q_{-c_1}Q_{-c_2}\frac{\operatorname{Tr}\tilde{c}^2}{4} = \operatorname{conj}\sum_{c\in l[0,0]} Q_{c_1}Q_{c_2}\frac{\operatorname{Tr}\tilde{c}^2}{4} = \overline{\alpha_l}\,.$$

This and analogous computations imply that $\mathsf{wi}_{2,-l} = \overline{\mathsf{wi}_{2,l}}$ and $\mathsf{wi}_{3,-l} = \overline{\mathsf{wi}_{3,l}}$.

More generally the summands of the Q-sums in the small partial wave invariants $\mathsf{wi}_{2,l}$ to $\mathsf{wi}_{5,l}$ are all real, because all imaginary units i, abbreviated with the tilde of $\tilde{c} = 2\pi\mathrm{i}c$, occur in even order. Also, all $\tilde{c}_i$ appear either as pairs of the form $\tilde{c}_{i,j}$ or $\tilde{F}_k(\tilde{c}_i, \tilde{c}_j)$ or are applied to l as in $\tilde{c}_i(l)$. Therefore, if we change $c \mapsto -c$ and $l \mapsto -l$, the summands of the Q-sums remain unchanged.

So for all Q-sums we have

$$\begin{aligned}\sum_{c\in(-l)[\dots]}^{Q} s(c,l) = \sum_{c\in(-l)[\dots]} Q_c s(c,l) &= \sum_{c\in l[\dots]} Q_{-c}s(-c,-l)\\ &= \sum_{c\in l[\dots]} \overline{Q_c}s(c,l) = \operatorname{conj}\sum_{c\in l[\dots]}^{Q} s(c,l)\,.\end{aligned}$$

It follows that $\mathsf{wi}_{k,-l} = \overline{\mathsf{wi}_{k,l}}$ for $k = 2, \dots, 5$. □

Lemma 5.10. If $\mathcal{L}$ is two-dimensional or if $\mathcal{L}$ is nondegenerate, then $|\tilde{F}l|^2$ does not depend on the choice of lattice vector of fixed length $|l| = d$.

Proof. If $\mathcal{L}$ is nondegenerate, then $|l'| = d = |l|$ implies $l' = \pm l$ and then $|\tilde{F}l|^2 = |\tilde{F}l'|^2$. If $\mathcal{L}$ is two-dimensional, let e_1 and e_2 denote the standard basis vectors of $\mathbb{R}^2$ and write $l = l_1e_1 + l_2e_2$. Then,

$$\begin{aligned}|\tilde{F}l|^2 = |\tilde{F}l(e_1)|^2 + |\tilde{F}l(e_2)|^2 &= |\tilde{F}(l_1e_1 + l_2e_2, e_1)|^2 + |\tilde{F}(l_1e_1 + l_2e_2, e_2)|^2\\ &= l_2^2|\tilde{F}(e_2,e_1)|^2 + l_1^2|\tilde{F}(e_1,e_2)|^2 = |l|^2\cdot|\tilde{F}(e_1,e_2)|^2\,.\end{aligned}$$

Thus, $|\tilde{F}l|^2$ depends only on the length of l. □

Lemma 5.10 is not true in higher dimensions.

Example 5.11. Consider $\mathbb{R}^4$ with the lattice spanned by the four standard basis vectors $\mathcal{L} = \mathbb{Z}(U_1, U_2, V_1, V_2) \coloneqq \mathbb{Z}(e_1, e_2, e_3, e_4)$. Choose the Chern factors

$$r_1 = F(U_1, V_1) \coloneqq 1 \qquad \text{and} \qquad r_2 = F(U_2, V_2) \coloneqq 2\,.$$

$U_1, U_2 \in \mathcal{L}$ are two lattice vectors of equal length but

$$|FU_1|^2 = |F(U_1, V_1)|^2 = 1 \qquad \text{and} \qquad |FU_2|^2 = |F(U_2, V_2)|^2 = 4 \neq 1\,.$$

This example might seem to suggest that Lemma 5.10 holds if we assume that all Chern factors are equal. This is not the case, however. Consider again $\mathbb{R}^4$ with the slightly modified lattice basis $V_2 := e_4/2$ and with Chern factors all equal to 1. Then, again $U_1, U_2 \in \mathcal{L}$ are two lattice vectors of equal length $|U_1| = 1 = |U_2|$ but the corresponding norms $|FU_i|$ are not equal:

$$\begin{aligned} &|FU_1|^2 = |F(U_1, V_1)|^2 = 1 \qquad \text{but} \\ &|FU_2|^2 = |F(U_2, e_4)|^2 = 4|F(U_2, e_4/2)|^2 = 4|F(U_2, V_2)|^2 = 4 \neq 1\,. \end{aligned}$$

If Lemma 5.10 does hold, further simplifications of the wave invariants are possible: We can multiply lower invariants by factors $|\tilde{F}l|$ and subtract those from higher invariants, because those factors do not, in the two-dimensional or nondegenerate case, depend on the choice of lattice vector $l \in \mathcal{L}$ with $|l| = d$.

Recall that the *frequency support* of the potential Q is given by

$$\mathcal{L}'_Q := \{c \in \mathcal{L}' \mid Q_c \neq 0\}\,.$$

Definition 5.12. We call

$$\mathcal{L}_Q := \{l \in \mathcal{L} \mid Q_{Fl} \neq 0\} \subset \mathcal{L}$$

the *lattice support* of the potential Q. We say that *frequencies* of Q are *on the lattice* if

$$F\mathcal{L}_Q = \mathcal{L}'_Q\,.$$

In other words, there are no $c \in \mathcal{L}'_Q \backslash F\mathcal{L}_Q$. Further, we say that the lattice support $\mathcal{L}_Q$ of a potential Q is *nondegenerate* if for $l, k \in \mathcal{L}_Q$

$$|l| = |k| \qquad \text{implies} \qquad l = \pm k\,.$$

Theorem 5.13. For all flat tori $M := \mathbb{R}^{2m}/\mathcal{L}$ with a Hermitian line bundle given by the Chern factors $(r_1, \ldots, r_m)$ and any translation-invariant connection given by a and any potential Q we have that if the lattice support $\mathcal{L}_Q$ is nondegenerate or M is two-dimensional, then for $k = 2, 3$ the simpler wave invariants

$$\mathsf{wi}^{\mathrm{s}}_{k,d}(a, Q) = \sum_{|l|=d} E_a(l)\sigma_l \cdot \mathsf{wi}^{\mathrm{s}}_{k,l}(Q)$$

given by

$$\mathsf{wi}^s_{2,l}(Q) \coloneqq \mathsf{wi}_{2,l}(Q) - \frac{|\tilde{F}l|^2}{6}\mathsf{wi}_{1,l}(Q) = \sum_{c\in I[0,0]}^{Q} 1$$

$$\mathsf{wi}^s_{3,l}(Q) \coloneqq \mathsf{wi}_{3,l}(Q) - \frac{|\tilde{F}l|^4}{48}\mathsf{wi}_{1,l}(Q) = -\sum_{c\in I[0,0]}^{Q} \frac{\operatorname{Tr}\tilde{c}^2}{4} + \sum_{c\in I[c_1,-c_1]}^{Q} \frac{6\tilde{c}_{1,2}}{\tilde{c}_1(l)^2} + \sum_{c\in I[0,0,0]}^{Q} 1$$

are also spectral invariants for all $d \in |\mathcal{L}|$.

Proof. If $\mathcal{L}$ is two-dimensional then Lemma 5.10 gives that neither $|\tilde{F}l|^2$ nor $|\tilde{F}l|^4$ depend on the choice of lattice vector $l \in \mathcal{L}$ of length $|l| = d$. If $\mathcal{L}_Q$ is nondegenerate then $|\tilde{F}l|^2 Q_{-Fl}$ and $|\tilde{F}l|^4 Q_{-Fl}$ depend only on $|l|$ since $Q_{-Fl} = 0$ for $l \notin \mathcal{L}_Q$. □

Remark 5.14. The signature σ_l of $l \in \mathcal{L}$ was defined as $\sigma_l = e_l(l/2) = \mathrm{e}^{\pi \mathrm{i} w_l(l)} = \mathrm{e}^{\pi \mathrm{i} \sum_{i=1}^{m} r_i u^i(l) v^i(l)}$. If $\mathcal{L}$ is nondegenerate, we must have $\sigma_l = \sigma_{l'}$ provided $|l| = |l'|$. Also, since $r_i \,|\, r_{i+1}$, it follows that if r_1 is even, then $\sigma_l = 1$ for all $l \in \mathcal{L}$. In both cases the value of σ_l does not depend on the choice of $l \in \mathcal{L}$ with a given length $|l| = d$. The signature σ_l can thus be dropped in the wave invariants.

However, this does not hold in general. Consider the lattice $\mathcal{L}$ where (a part of) the Chern basis is given by $U_1 \coloneqq e_1$ and $V_1 \coloneqq e_2/\sqrt{3}$. Set $r_1 \coloneqq 1$. Then,

$$|U_1 + V_1|^2 = 1 + 1/3 = 4/3 = |2V_1|^2$$

but $w_{U_1+V_1}(U_1 + V_1) = r_1 \cdot 1 \cdot 1 = 1$ and $w_{2V_1}(2V_1) = r_1 \cdot 0 \cdot 2 = 0$. Therefore, the value of the signature can vary within the set of lattice vectors of length $2/\sqrt{3}$,

$$\sigma_{U_1+V_1} = -1 \qquad \text{but} \qquad \sigma_{2V_1} = 1\,.$$

5.2 Correctness

Given the complexity of the MATHEMATICA notebook of Appendix D we might ask if the resulting wave invariants are correct. Two sources of errors seem conceivable: there might be a programming error in the notebook or the computer algebra system MATHEMATICA itself could be faulty. An example for latter has been given in [DPV14]. Is there at least some heuristic way to test for errors of the resulting wave invariants?

Apart from computing simple subexpressions of the partial wave invariants and comparing them to the computational result we can also look for transplantations as in Chapter 2 and test if the computed wave invariants reflect the implied isospectralities. In fact, it is not hard to show that if a triple

$(Q, a, b) \in C^\infty(M) \times \mathbb{R}^{n'} \times \mathbb{R}^{n'}$ is of type (M) or of type (P) then not only are $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_b + Q$ isospectral but we indeed have

$$\mathsf{wi}_{k,d}(a, Q) = \mathsf{wi}_{k,d}(b, Q) \qquad \text{for } k = 1, \dots, 5.$$

Also, we can decide not to use the necessary conditions to speed up the computation of the wave invariants and instead check if they are satisfied by the results. This is computationally very expensive, of course, and is done in the MATHEMATICA notebook of Appendix D.

There are also other examples that we will discuss now.

Example 5.15. It is clear that if two connections $a, b \in \mathbb{R}^{n'}$ are isospectral with respect to some smooth potential then they are also isospectral with respect to $Q + q$ for any constant $q \in \mathbb{R}$.

In other words, we should then have $\mathsf{wi}_{k,d}(a, Q+q) - \mathsf{wi}_{k,d}(b, Q+q) = 0$ and this is indeed the case. We can show this by differentiating $\mathsf{wi}_{k,l}(Q)$ for the computed invariants $k = 1, \dots, 5$ with respect to Q_0. This differential is not zero but one can show that it is a linear combination of lower order partial wave invariants. For example,

$$\partial/(\partial Q_0)\mathsf{wi}_{2,l}(Q) = 2Q_{-Fl} = 2\mathsf{wi}_{1,l}(Q)\,.$$

Since $\mathsf{wi}_{1,d}(a, Q+q) - \mathsf{wi}_{1,d}(b, Q+q) = 0$ (as $d \neq 0$) for all q it follows inductively that

$$\partial/(\partial Q_0)\Big(\mathsf{wi}_{k,d}(a, Q) - \mathsf{wi}_{k,d}(b, Q)\Big) = 0 \qquad \text{for } k = 2, \dots, 5$$

and thus

$$\mathsf{wi}_{k,d}(a, Q+q) - \mathsf{wi}_{k,d}(b, Q+q) = \mathsf{wi}_{k,d}(a, Q) - \mathsf{wi}_{k,d}(b, Q) = 0$$

for $k = 1, \dots, 5$, as desired.

Example 5.16. The map $s \mapsto \check{s}$ with $\check{s}(x) := s(-x)$ is a transplantation between $\Delta_a^{\mathrm{D}} + Q$ and $\Delta_{-a}^{\mathrm{D}} + \check{Q}$ and thus those two operators must be isospectral, see [Ber17, Example 6.2] or, for the case $a = 0$, [GGKW08, Remarks 2.19 (v)]. This transplantation is reflected in the first five wave invariants: Note first that for $c \in l[\mathfrak{c}_1, \dots, \mathfrak{c}_h]$ we have $-c \in (-l)[\mathfrak{c}_1, \dots, \mathfrak{c}_h]$ and $(\check{Q})_c = Q_{-c}$. Hence, for $k = 1, \dots, 5$,

$$\begin{aligned}\mathsf{wi}_{k,d}(-a, \check{Q}) &= \sum_{|l|=d} E_{-a}(l)\sigma_l \mathsf{wi}_{k,l}(\check{Q}) \\ &= \sum_{|-l|=d} E_{-a}(-l)\sigma_{-l}\mathsf{wi}_{k,-l}(\check{Q}) = \sum_{|l|=d} E_a(l)\sigma_l \mathsf{wi}_{k,l}(Q) = \mathsf{wi}_{k,d}(a, Q)\,,\end{aligned}$$

because in the first five wave invariants all c appear in pairs or as $c(l)$.

Chapter 6

Applications

In this Chapter we will use the wave invariants to obtain positive spectral results. In Chapter 2 we have constructed transplantations and thus an isospectrality relation if two connections are of type (P) or of type (M) with respect to some potential. Here we will show for certain, sufficiently simple potentials that conversely two connections must be of either type if they are isospectral. If the involved lattices are degenerate we will give an example where isospectrality holds exactly if the two connections are merely of mixed type. By an explicit construction we will demonstrate that we can find potentials such that the set of isospectral translation-invariant connections is a union of an arbitrary given number of subspaces with an arbitrary given number of degrees of freedom.

After that we will use the necessary conditions to draw more general conclusions about the wave invariants. This will imply limitations of the information contained in the first N wave invariants for $N \in \mathbb{N}$: We can always find lattices and potentials such that an arbitrary large number of wave invariants vanishes.

Additionally, we know that for constant potentials all translation-invariant connections are isospectral. We conjecture that the converse is also true. We show that if all connections are isospectral then all partial wave invariants must vanish. This in turn leads to the existence of nonisospectral connections for at least some classes of potentials.

6.1 Hearing Types

In Chapter 2 we have shown that two translation-invariant connections given by $a, b \in \mathbb{R}^{n'}$ whose triple (Q, a, b) is either of type (M) or of type (P) (recall Definition 2.13) with respect to the curvature form F are isospectral. In this chapter we will use the wave invariants to show the converse of this statement

for certain potentials Q. Note that Theorem 2.14 requires that the tuple (Q, a, b) is entirely of either type to imply isospectrality and cannot, in general, be applied if (Q, a, b) is only of mixed type.

By Theorem 6.20 below the first k wave invariants can vanish if the frequency support of the potential Q is "small" and $F(\mathcal{L})$ "large". For this reason, we consider potentials whose frequency support is *on the lattice* in this section.

Recall that the *frequency support* of the potential Q is given by

$$\mathcal{L}'_Q := \{c \in \mathcal{L}' \mid Q_c \neq 0\} .$$

and by Definition 5.12

$$\mathcal{L}_Q := \{l \in \mathcal{L} \mid Q_{Fl} \neq 0\} \subset \mathcal{L}$$

is the *lattice support* of the potential Q. We say that the *frequencies* of Q are *on the lattice* if $F\mathcal{L}_Q = \mathcal{L}'_Q$. Further, we say that the lattice support $\mathcal{L}_Q$ of a potential Q is *nondegenerate* if for $l, k \in \mathcal{L}_Q$

$$|l| = |k| \qquad \text{implies} \qquad l = \pm k .$$

Note that because Q is real-valued $l \in \mathcal{L}_Q$ implies $-l \in \mathcal{L}_Q$. If all the Chern invariant factors are one, $r = \mathbb{1}$, then $F\mathcal{L} = \mathcal{L}'$ and the frequencies of any potential are automatically on the lattice. If the lattice $\mathcal{L}$ itself is nondegenerate then so is the lattice support of any potential.

We begin with a technical reformulation of Definition 2.13.

Lemma 6.1. Given a potential Q and some $l \in \mathcal{L}_Q$ then two connections a and b are of type (M) or of type (P) with respect to Fl exactly if

$$\operatorname{Re}\Big(\big(E_a(l) - E_b(l)\big)Q_{-Fl}\Big) = 0 .$$

Proof. It is easy to see that (Q, a, b) is of type (M) with respect to Fl if and only if $E_a(l) = E_b(l)$, so the equation follows. If it is of type (P) then

$$Q_{Fl} = Q_{-Fl} E_{-Fl}(G(a + b))$$

and, because $Fl(G(a + b)) = F(l, G(a + b)) = -F(G(a + b), l) = -(a + b)(l)$, we have

$$\begin{aligned} \alpha := \big(E_a(l) - E_b(l)\big)Q_{-Fl} &= \big(E_a(l) - E_b(l)\big)Q_{Fl}E_{Fl}(G(a + b)) \\ &= \big(E_a(l) - E_b(l)\big)Q_{Fl}E_{-a-b}(l) = -\big(E_{-a}(l) - E_{-b}(l)\big)Q_{Fl} = -\overline{\alpha} , \end{aligned}$$

which implies $\operatorname{Re}\alpha = 0$.

Conversely, if $\operatorname{Re}\alpha = 0$ then

$$\Big(E_a(l) - E_b(l)\Big)Q_{-Fl} = \Big(E_{-b}(l) - E_{-a}(l)\Big)Q_{Fl}\,.$$

If we assume that (Q,a,b) is not of type (M) with respect to Fl then $E_b(-l) - E_a(-l) \neq 0$ and

$$Q_{Fl} = Q_{-Fl}\cdot\frac{E_a(l)-E_b(l)}{E_{-b}(l)-E_{-a}(l)} = Q_{-Fl}E_{a+b}(l) = Q_{-Fl}E_{-Fl}(G(a+b))$$

and (Q,a,b) are of type (P) with respect to Fl. □

Lemma 6.2. If Q is a potential with frequencies on the lattice and whose lattice support is nondegenerate then isospectrality of a and b with respect to Q implies that (Q,a,b) is of mixed type.

Proof. We use the first small wave invariant $\mathsf{wi}_{1,|l|}(a,Q)$ given in Theorem 5.8. The corresponding partial invariants are

$$\mathsf{wi}_{1,l}(Q) = Q_{-Fl} \qquad \text{for any } l \in \mathcal{L}.$$

We have assumed that the lattice support $\mathcal{L}_Q$ is nondegenerate, which implies for all $l \in \mathcal{L}_Q$

$$\begin{aligned}\mathsf{wi}_{1,|l|}(a,Q) &= E_a(l)\sigma_l\cdot\mathsf{wi}_{1,l}(Q) + E_a(-l)\sigma_{-l}\cdot\mathsf{wi}_{1,-l}(Q)\\ &= \sigma_l\Big(E_a(l)Q_{-Fl} + E_a(-l)\cdot Q_{Fl}\Big) = 2\sigma_l\operatorname{Re}(E_a(l)Q_{-Fl})\,,\end{aligned}$$

since the sign $\sigma_l \in \{\pm 1\}$ is independent of the sign of l. If a and b are isospectral we have

$$\mathsf{wi}_{1,|l|}(a,Q) - \mathsf{wi}_{1,|l|}(b,Q) = 2\sigma_l\operatorname{Re}\Big(E_a(l) - E_b(l)\Big)Q_{-Fl} = 0$$

and Lemma 6.1 implies that (Q,a,b) is of type (M) or of type (P) with respect to Fl.

Because we assumed that the frequency support of Q is on the lattice, $\mathcal{L}'_Q = F\mathcal{L}_Q$, it follows that (Q,a,b) must be of one the two types with respect to each $c \in \mathcal{L}'_Q$. Thus, (Q,a,b) is of mixed type. □

Because the type of (Q,a,b) with respect to c and $-c$ is the same we have the following corollary.

Corollary 6.3. If Q has the simplest nontrivial frequency support on the lattice,

$$\mathcal{L}'_Q = \{\pm Fl\} \qquad \text{for some } l \in \mathcal{L}\backslash\{0\},$$

then the hypotheses of Lemma 6.2 are obviously satisfied; thus a and b are isospectral with respect to the potential Q if and only if (Q,a,b) is either of type (P) or of type (M).

We can also use Lemma 6.2 to construct potentials that spectrally determine the connections to any degree we choose. Recall that by Proposition 1.23, connections differing by elements of the dual lattice $\mathcal{L}'$ are always isospectral.

Theorem 6.4. For any lattice $\mathcal{L}$ and any two natural numbers $N_1 \in \mathbb{N}$ and $0 \leq N_2 < n$ we can find a smooth real-valued potential $Q \in C^\infty(M)$ such that for any $a \in \mathbb{R}^{n'}$ the set $\mathrm{Iso}_Q(a)$ of translation-invariant connections in $\mathbb{R}^{n'}/\mathcal{L}'$ which are isospectral to a with respect to Q consists of exactly N_1 smooth families of dimension N_2.

More precisely, with $(X_1, \ldots, X_n) \coloneqq (U_1, \ldots, U_m, V_1, \ldots, V_m)$ we can choose Q such that for all connections $a \in \mathbb{R}^{n'}$

$$\mathrm{Iso}_Q(a) = \left\{ [a + \frac{i}{N_1} X^1 + \alpha_1 X^{n-N_2+1} + \cdots + \alpha_{N_2} X^n] \mid i \in \mathbb{Z},\ \alpha_1, \ldots, \alpha_{N_2} \in \mathbb{R} \right\}$$

within $\mathbb{R}^{n'}/\mathcal{L}'$.

In particular, letting $N_1 \coloneqq 1$ and $N_2 \coloneqq 0$ there exists a potential Q such that each translation-invariant connections $[a] \in \mathbb{R}^{n'}/\mathcal{L}'$ are spectrally determined by $\mathrm{Spec}_a(Q, \omega)$.

Proof. Let $Y_1 \coloneqq N_1 X_1$ and $Y_i \coloneqq X_i$ for $i > 1$. The potential Q shall have its frequency support on the lattice and thus we choose a lattice support as follows. Let

$$\mathcal{L}_+ \coloneqq \left\{ p_{1,j} Y_1, \ldots, p_{n-N_2,j} Y_{n-N_2} \mid j = 1, 2, 3 \right\},$$

where the $p_{i,j}$ are prime numbers (or 1) such that all elements of $\mathcal{L}_+$ are of a different length. Now, the lattice support of Q shall be

$$\mathcal{L}_Q \coloneqq -\mathcal{L}_+ \cup \mathcal{L}_+ .$$

Since we have constructed this lattice support to be nondegenerate, we can apply Lemma 6.2: If two translation-invariant connections a and b are isospectral with respect to Q then (Q, a, b) must be of mixed type.

In the following we make use of the alternative description of the types given in Remark 2.16. We choose the phases $\phi_{Fp_{i,j}Y_i}(Q)$ of the Fourier coefficients of Q such that for each $i \in \{1, \ldots, n - N_2\}$:

$$\begin{aligned}
&2p_{i,1}\phi_{Fp_{i,2}Y_i} \not\equiv 2p_{i,2}\phi_{Fp_{i,1}Y_i}, \\
&2p_{i,1}\phi_{Fp_{i,3}Y_i} \not\equiv 2p_{i,3}\phi_{Fp_{i,1}Y_i}, \\
&2p_{i,2}\phi_{Fp_{i,3}Y_i} \not\equiv 2p_{i,3}\phi_{Fp_{i,2}Y_i} \qquad \text{modulo } \mathbb{Z}.
\end{aligned}$$

If (Q, a, b) were of type (P) with respect to two of the three lattice vectors $p_{i,j}Y_j$, say $j = 1$ and $j = 2$, then we would have

$$[2\phi_{Fp_{i,j}Y_i}] = [F'(F(p_{i,j}Y_i), a + b)] = [-(a + b)(p_{i,j}Y_i)] \qquad \text{for } i = 1, 2$$

and by $-p_{i,2} \cdot (a+b)(p_{i,1}Y_i) = -p_{i,1} \cdot (a+b)(p_{i,2}Y_i)$ this would imply that

$$[2p_{i,2}\phi_{Fp_{i,1}Y_i}] = [2p_{i,1}\phi_{Fp_{i,2}Y_i}]\,.$$

This, however, is not possible by the choice of phases above. Thus, if a and b are isospectral with respect to Q then (Q,a,b) must be of type (M) with respect to at least two of the three vectors $p_{i,j}Y_i$ for all $i \in \{1,\dots,n-N_2\}$.

Assuming again that this is the case for $j=1$ and $j=2$ it follows that

$$(a-b)(p_{i,1}Y_i) \in \mathbb{Z} \qquad \text{and} \qquad (a-b)(p_{i,2}Y_i) \in \mathbb{Z}\,.$$

Since all $p_{i,j}$ are prime numbers or 1, we have that

$$(a-b)(Y_i) \in \mathbb{Z} \qquad \text{for all } i \in \{1,\dots,n-N_2\}.$$

In particular, if a and b are isospectral with respect to Q then (Q,a,b) must be of type (M). Conversely, if (Q,a,b) is of type (M) then a and b are isospectral by Theorem 2.14.

Thus, a and b are isospectral with respect to Q if and only if

$$(a-b)(N_1X_1) \in \mathbb{Z} \qquad \text{and} \qquad a(X_i) \equiv b(X_i) \quad \text{for all } 1 < i \le n-N_2. \qquad \square$$

A potential satisfying the conditions of the proof of Theorem 6.4 is given in the following example.

Example 6.5. Let us consider the two-dimensional lattice $\mathcal{L}$ given by the lattice basis $U_1 \coloneqq e_1$ and $V_1 \coloneqq e_2$. Let $r_1 \coloneqq 1$ and $N_1 \coloneqq 1$, $N_2 \coloneqq 1$. The lattice vectors U_1, $2U_1$ and $3U_1$ have different lengths and $\mathcal{L}_Q \coloneqq \pm\{U_1, 2U_1, 3U_1\}$ shall be the lattice support of Q. Let $\phi_{FU_1}(Q) \coloneqq 0$, $\phi_{F(2U_1)}(Q) \coloneqq 3/4$ and $\phi_{F(3U_1)}(Q) \coloneqq 1/4$, such that the phases satisfy the inequations (modulo $\mathbb{Z}$) of the proof of Theorem 6.4. The corresponding Fourier coefficients of the potential can have arbitrary positive absolute values, but $1/2$ is convenient.

$$Q_{FU_1} = 1/2\,, \quad Q_{F(2U_1)} = -\mathrm{i}/2 \qquad \text{and} \qquad Q_{F(3U_1)} = \mathrm{i}/2\,.$$

By $r_1 = 1$ we have $FU_1 = V^1$ and the potential is then (in standard coordinates) given by

$$Q(u,v) = \cos(2\pi v) - \sin(4\pi v) + \sin(6\pi v)\,.$$

For this potential two connections a and b are isospectral exactly if $(a-b)(U_1) = a_1 - b_1 \in \mathbb{Z}$. In particular, $\mathrm{Iso}_Q(a) = \left\{[a + \alpha V^1] \mid \alpha \in \mathbb{R}\right\}$.

Alternatively, if we let $N_2 \coloneqq 0$ and choose the potential

$$\begin{aligned} Q(u,v) \coloneqq{}& \cos(2\pi v) - \sin(4\pi v) + \sin(6\pi v) \\ &+ \cos(2\pi u) - \sin(4\pi u) + \sin(6\pi u) \end{aligned}$$

then each $[a] \in \mathbb{R}^{n'}/\mathcal{L}'$ is determined by $\mathrm{Spec}_a(Q,\omega)$.

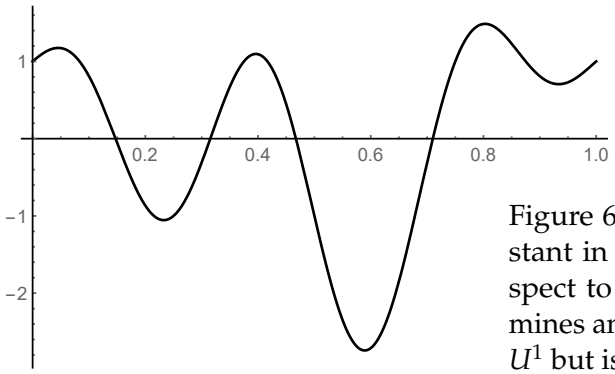


Figure 6.1: The potential that is constant in u and whose graph with respect to v is shown spectrally determines any connection in the direction U^1 but is deaf in the direction V^1.

Given nondegeneracy of $\mathcal{L}_Q$ and Q with all frequencies on the lattice we can so far only conclude that (Q, a, b) must be of mixed type, if a and b are isospectral with respect to Q. In Theorem 6.4 we have chosen the phases of the Fourier coefficents of Q in such a way that only type (M) is possible.

However, the higher wave invariants allow us, in some cases, to link the types of the different frequencies, such that we can show that isospectrality implies not just that (Q, a, b) is of mixed type but that it must be of type (M) or of type (P) without any assumptions on the phases of Q.

For that we need to compute Q-sums over various cases, recall Definition 5.1. We need those parts of the cases on which the potential Q has nonzero Fourier coefficients. Recall that we have defined

$$Q_c \coloneqq Q_{c_1} \cdots Q_{c_q} \qquad \text{for } c \in \mathcal{L}'^q.$$

Definition 6.6. Let $M \coloneqq \mathbb{R}^n / \mathcal{L}$ denote a flat torus, $l \in \mathcal{L}$ and $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q] \subset \mathcal{L}'^q$ some case. For a given potential Q on M we denote by

$$l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_Q \coloneqq \left\{ c \in l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q] \mid Q_c \neq 0 \right\}$$

the *supported* subset of the given case. We say a case is supported if its supported subset is not empty.

It is clear from Definition 5.5 that only the supported subset of a case may contribute via its Q-sum and if a case is unsupported then its Q-sum vanishes.

Lemma 6.7. Let Q denote a potential on the torus $M = \mathbb{R}^n / \mathcal{L}$ that satisfies the following assumptions:

(1) The frequencies of Q are on the lattice (Definition 5.12) and its lattice support $\mathcal{L}_Q$ is nondegenerate.

(2) $\mathcal{L}_Q + \mathcal{L}_Q \coloneqq \left\{ l_1 + l_2 \mid l_1, l_2 \in \mathcal{L}_Q \right\}$ is maximal and nondegenerate.

(3) There is an enumeration $\mathcal{L}_Q = \{l_1, -l_1, l_2, -l_2 \ldots\}$ such that $Fl_i(l_{i+1}) = 0$.

Then two connections a and b are isospectral with respect to Q if and only if (Q, a, b) is of type (M) or of type (P).

Here, $\mathcal{L}_Q + \mathcal{L}_Q$ is assumed to be maximal in the sense that if $l_1 + l_2 = k_1 + k_2 \neq 0$ then $\{l_1, l_2\} = \{k_1, k_2\}$.

Proof. Let a and b be isospectral with respect to Q. It follows from condition (1) and Lemma 6.2 that (Q, a, b) is of mixed type. It remains to show that (Q, a, b) is of the same type with respect to all Fl_i. So we assume that there is an $l_i \in \mathcal{L}_Q$ such that (Q, a, b) is of type (P) with respect to Fl_i but of type (M) with respect to Fl_{i+1}. The reverse case is treated in the same way. We can use the second wave invariant with respect to $l := l_i + l_{i+1} \in \mathcal{L}_Q + \mathcal{L}_Q$ to obtain a link between those two (dual) lattice vectors.

We have assumed that $\mathcal{L}_Q + \mathcal{L}_Q$ is nondegenerate and therefore

$$\mathsf{wi}_{2,|l|}(a, Q) = \sigma_l\Big(E_a(l)\mathsf{wi}_{2,l}(Q) + E_a(-l)\mathsf{wi}_{2,-l}(Q)\Big).$$

Since $\mathcal{L}_Q$ is nondegenerate we can use the simple partial wave invariant of Theorem 5.13

$$\mathsf{wi}^{\mathrm{s}}_{2,l}(Q) = \sum_{c \in l[0,0]}{}^{Q} 1 \qquad \text{instead of } \mathsf{wi}_{2,l}(Q).$$

Let us compute $l[0,0]_Q$. An element $c \in l[0,0]_Q$ must not only satisfy $c_1 + c_2 = -Fl = -Fl_i - Fl_{i+1}$ but also $c_1, c_2 \in \mathcal{L}'_Q = F\mathcal{L}_Q$. Thus, there are $k_1, k_2 \in \mathcal{L}_Q$ with $c_i = Fk_i$. The maximality of $\mathcal{L}_Q + \mathcal{L}_Q$ implies that there is exactly one such pair of lattice vectors: $\{k_1, k_2\} = \{-l_i, -l_{i+1}\}$. Assumption (3) further assures that

$$F(-l_i)(l) = -Fl_i(l_i + l_{i+1}) = -Fl_i(l_{i+1}) = 0 = F(-l_{i+1})(l)\,.$$

Therefore,

$$l[0,0]_Q = \{(-Fl_i, -Fl_{i+1}), (-Fl_{i+1}, -Fl_i)\}\,.$$

Having computed this case it is easy to calculate the second simple partial wave invariant:

$$\mathsf{wi}^{\mathrm{s}}_{2,l}(Q) = 2Q_{-Fl_i}Q_{-Fl_{i+1}}$$

If a and b are isospectral then their simple wave invariants must be equal.

$$\begin{aligned}\mathsf{wi}^{\mathrm{s}}_{2,|l|}(a, Q) &= 2\sigma_l\Big(E_a(l)Q_{-Fl_i}Q_{-Fl_{i+1}} + E_a(-l)Q_{Fl_i}Q_{Fl_{i+1}}\Big)\\ &= 2\sigma_l\Big(E_b(l)Q_{-Fl_i}Q_{-Fl_{i+1}} + E_b(-l)Q_{Fl_i}Q_{Fl_{i+1}}\Big) = \mathsf{wi}^{\mathrm{s}}_{2,|l|}(b, Q)\end{aligned}$$

Rearranging yields

$$\Big(E_a(-l) - E_b(-l)\Big)Q_{Fl_i}Q_{Fl_{i+1}} = \Big(E_b(l) - E_a(l)\Big)Q_{-Fl_i}Q_{-Fl_{i+1}}\,.$$

Since we have assumed that (Q, a, b) is of type (M) with respect to Fl_{i+1}, we have

$$1 = E_{Fl_{i+1}}(G(a-b)) = E_{b-a}(l_{i+1})\,.$$

So, if we have that

$$E_a(-l) - E_b(-l) = 0 \qquad \text{or equivalently} \qquad E_{b-a}(l_i + l_{i+1}) = 1\,,$$

then

$$E_{b-a}(l_i) = 1\,.$$

Hence, (Q, a, b) is also of type (M) with respect to Fl_i.

On the other hand, if $E_a(-l) - E_b(-l) \neq 0$ then

$$\frac{Q_{Fl_i} Q_{Fl_{i+1}}}{Q_{-Fl_i} Q_{-Fl_{i+1}}} = \frac{E_b(l) - E_a(l)}{E_a(-l) - E_b(-l)} = E_{a+b}(l) = E_{a+b}(l_i) \cdot E_{a+b}(l_{i+1})\,.$$

The assumption that (Q, a, b) is of type (P) with respect to Fl_i, that is $Q_{Fl_i}/Q_{-Fl_i} = E_{a+b}(l_i)$, implies

$$\frac{Q_{Fl_{i+1}}}{Q_{-Fl_{i+1}}} = E_{a+b}(l_{i+1})\,.$$

In this case, (Q, a, b) is also of type (P) with respect to Fl_{i+1}. Either way, (Q, a, b) is of the same type with respect to Fl_i and Fl_{i+1}.

Overall, we have used the second wave invariant to show that (Q, a, b) must be of the same type with respect to all $c \in \mathcal{L}'_Q$. Therefore, (Q, a, b) must be of type (P) or of type (M). □

The question arises whether we can find lattices and potentials such that the conditions of Lemma 6.7 are satisfied.

Example 6.8. If we assume that the lattice $\mathcal{L}$ itself is nondegenerate then $\mathcal{L}_Q$ and $\mathcal{L}_Q + \mathcal{L}_Q$ are both automatically nondegenerate as well. If we choose the lattice support of Q to be contained in the span of $\{U_i\}_{i\in I} \cup \{V_i\}_{i\in J}$ such that $I \cap J = \emptyset$ then we have $Fl(k) = 0$ for all $l, k \in \mathcal{L}_Q$.

It remains to assure that $\mathcal{L}_Q + \mathcal{L}_Q$ is maximal. For example, we can choose a potential Q with the finite lattice support

$$\mathcal{L}_Q = \{\pm U_1, \ldots, \pm U_k\}$$

but potentials with infinite lattice support can also easily be found. (Q is smooth if the Fourier coefficients Q_c go to zero sufficiently fast for increasing $|c|$.) A possible choice of lattice support is

$$\mathcal{L}_Q = \left\{\pm(kU_1 + k^2 U_2) \mid k \in \mathbb{N}\right\}\,.$$

In the latter case $\mathcal{L}_Q + \mathcal{L}_Q$ is maximal because

$$(kU_1 + k^2U_2) + (hU_1 + h^2U_2) = (sU_1 + s^2U_2) + (tU_1 + t^2U_2)$$

implies $(k+h, k^2+h^2) = (s+t, s^2+t^2)$ and if we solve for s and t we have only the two solutions $(s,t) = (k,h)$ and $(s,t) = (h,k)$. Additionally, $(k+h, k^2+h^2) = (s-t, s^2-t^2)$ implies $k^2+h^2+t^2 = s^2 = (k+h+t)^2$ and thus has no solutions for $k, h, s, t \in \mathbb{N}$.

Example 6.9. We can also find potentials with infinite lattice support such that $\mathcal{L}_Q + \mathcal{L}_Q$ is maximal in dimension 2. Let $\mathcal{L}$ be any lattice, nondegenerate or not, and Q a potential such that

$$\mathcal{L}_Q \subset \{\pm k_1 U_1, \pm k_2 U_1, \pm k_3 U_1 \dots\}$$

with $3k_i < k_{i+1}$. If we choose four elements from this set with $k_{i_1}, k_{i_2}, k_{i_3} < k_{i_4}$ we have $k_{i_1} + k_{i_2} + k_{i_3} < k_{i_4}$ and we can never have $\pm k_{i_1} \pm k_{i_2} = \pm k_{i_3} \pm k_{i_4}$ for any choice of signs. Thus, $\mathcal{L}_Q + \mathcal{L}_Q$ is maximal.

Example 6.10. More explicitly, if $\mathcal{L}$ is nondegenerate and of dimension greater than 2, we can choose the smooth potential

$$Q(u,v) = \cos 2\pi r_1 v^1 + \cos 2\pi r_2 v^2 \,,$$

which has the frequency support $\mathcal{L}'_Q = \{\pm r_1 V^1, \pm r_2 V^2\}$. The frequency support is on the lattice and the lattice support is

$$\mathcal{L}_Q = \{\pm U_1, \pm U_2\} \,.$$

The conditions of Lemma 6.7 are satisfied and thus then $\Delta^{\mathrm{D}}_a + Q$ and $\Delta^{\mathrm{D}}_b + Q$ are isospectral if and only if (Q, a, b) is of type (P) or of type (M).

Now, we consider the same scenario but assume that $Fl_i(l_{i+1}) \neq 0$. In this case it depends on the lattice and the curvature form F whether we can conclude that (Q, a, b) is of type (M) or of type (P). For simplicity we need to assume that there are only four lattice vectors $\pm l_1$ and $\pm l_2$ in the lattice support.

Lemma 6.12 below and the following examples show that it is possible to draw information from each of the first five wave invariants. The examples also demonstrate limits on the simplification of the wave invariants: Terms that are nonvanishing in examples cannot vanish in simplifications without additional assumptions.

For a more uniform formulation of the following lemma we make the following definition.

Definition 6.11. We extend the Definitions 3.7 and 5.3 of curvature traces F_k to $k = 0$ by setting

$$F_0(c,d) \coloneqq \operatorname{Tr} c \cdot d = c(e_i)d(e_i) \qquad \text{for } c,d \in \mathcal{L}'.$$

Lemma 6.12. Assume that the frequency support of the potential Q has four elements

$$\mathcal{L}'_Q = \{\pm Fl_1, \pm Fl_2\} \qquad \text{with } l_1, l_2 \in \mathcal{L}\backslash\{0\}.$$

We again set $l \coloneqq l_1 + l_2$ but assume that

$$Fl_1(l) = -Fl_2(l) \neq 0\,.$$

We assume the lattice support $\mathcal{L}_Q = \{\pm l_1, \pm l_2\}$ to be nondegenerate and additionally that there are only two vectors of length $|l_1 + l_2|$ within $\mathbb{Z}(l_1, l_2)$. If

$$F_0(Fl_1, Fl_2) \neq 0 \qquad \text{or} \qquad F_1(Fl_1, Fl_2) \neq 0 \qquad \text{or} \qquad F_2(Fl_1, Fl_2) \neq 0$$

then a and b are isospectral with respect to Q if and only if (Q, a, b) is of type (P) or of type (M).

Proof. Let a and b be isospectral with respect to Q. Since we have assumed that $\mathcal{L}_Q$ is nondegenerate and since Q has frequencies on the lattice by the choice of $\mathcal{L}'_Q$, we can apply Lemma 6.2 which implies that (Q, a, b) is of type (P) or type (M) for $\pm Fl_1$ and $\pm Fl_2$ separately. Again, we have to find a connection between the types of these dual lattice vectors by using higher wave invariants.

We study the (partial) wave invariants with respect to the lattice vectors $\pm l = \pm(l_1 + l_2)$. The wave invariants corresponding to $|l|$ are of the form $\sum_{|h|=|l|} E_a(h)\sigma_h \mathsf{wi}_{k,h}(Q)$ and there may be lattice vectors $h \in \mathcal{L}\backslash\{\pm l\}$ that are of the same length as $|l|$. However, for such an h the partial wave invariants $\mathsf{wi}_{k,h}(Q)$ must vanish: By assumption h is not an integral linear combination of l_1 and l_2. In particular, the definition of $\mathcal{L}'_Q$ implies $Q_{-Fh} = 0$. But we also have that for any case $h[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$

$$c \in h[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_Q \quad \text{implies per definitionem} \quad c_1 + \cdots + c_q = -Fh \quad \text{and} \quad c_1, \ldots, c_q \in \mathcal{L}'_Q\,.$$

Since the lattice support of the potentials under consideration is particularly simple we have $c_i \in \{\pm Fl_1, \pm Fl_2\}$ and thus $\alpha Fl_1 + \beta Fl_2 = -Fh$ for some $\alpha, \beta \in \mathbb{Z}$. Again, this is not possible because $\alpha l_1 + \beta l_2 \neq -h$ for all $\alpha, \beta \in \mathbb{Z}$. Thus,

$$h[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_Q = \emptyset \qquad \text{and} \qquad \mathsf{wi}_{k,h}(Q) = 0 \qquad \text{for all } k \in \{1 \cdots 5\}.$$

It follows that in order to compute $\mathsf{wi}_{k,|l|}(Q)$ we only need to compute the partial wave invariants $\mathsf{wi}_{k,\pm l}(Q)$. Note that $Q_{-Fl} = 0$ because $l \notin \{\pm l_1, \pm l_2\}$ by the assumption $Fl_i(l) \neq 0$. The latter also implies

$$l[\mathfrak{c}_1, \dots, \mathfrak{c}_q]_Q = \emptyset \qquad \text{whenever } \mathfrak{c}_i = 0 \text{ for at least one } i \in \{1, \dots, q\}\,.$$

Therefore $\mathsf{wi}_{1,\pm l}(Q) = \mathsf{wi}_{2,\pm l}(Q) = 0$.

Further, $l[0,0,0]_Q = \emptyset$ and

$$l[c_1, -c_1]_Q = \{(-Fl_1, -Fl_2), (-Fl_2, -Fl_1)\}\,.$$

Therefore,

$$\begin{aligned}\mathsf{wi}_{3,l}(Q) &= \sum_{c \in l[c_1,-c_1]}^{Q} \frac{6\tilde{c}_{1,2}}{\tilde{c}_1(l)^2} \\ &= Q_{-Fl_1} Q_{-Fl_2} \cdot 12 \frac{\mathrm{Tr}(Fl_1 \cdot Fl_2)}{Fl_1(l)^2} = Q_{-Fl_1} Q_{-Fl_2} \cdot 12 \frac{F_0(Fl_1 \cdot Fl_2)}{Fl_1(l)^2} \quad \text{and} \\ \mathsf{wi}_{3,-l}(Q) &= Q_{Fl_1} Q_{Fl_2} \cdot 12 \frac{F_0(Fl_1 \cdot Fl_2)}{Fl_1(l)^2}\,.\end{aligned}$$

Analogously to the second half of the proof of Lemma 6.7 we can conclude that $\pm Fl_1$ and $\pm Fl_2$ are of the same type if $F_0(Fl_1, Fl_2) \neq 0$.

If, on the other hand, $F_0(Fl_1, Fl_2) = 0$ then $\mathsf{wi}_{3,\pm l}(Q) = 0$ and we have to study the fourth invariant. Under our assumptions the fourth partial wave invariant simplifies to

$$\begin{aligned}\mathsf{wi}_{4,l}(Q) &= \sum_{c \in l[c_1,-c_1]}^{Q} 48 \frac{F_1(c_1, c_2)}{c_1(l)^3} = -Q_{-Fl_1} Q_{-Fl_2} \cdot \frac{96}{Fl_1(l)^3} F_1(Fl_1, Fl_2) \quad \text{and} \\ \mathsf{wi}_{4,-l}(Q) &= -Q_{Fl_1} Q_{Fl_2} \cdot \frac{96}{Fl_1(l)^3} F_1(Fl_1, Fl_2)\,,\end{aligned}$$

because $Q_{-Fl} = 0$, $l[0, c_2, -c_2]_Q = \emptyset$ and $l[0,0,0,0]_Q = \emptyset$. Again, the claim that $\pm Fl_1$ and $\pm Fl_2$ have the same type follows analogously to the second half of the proof of Lemma 6.7, provided $F_1(Fl_1, Fl_2) \neq 0$.

We now assume that both $F_0(Fl_1, Fl_2)$ and $F_1(Fl_1, Fl_2)$ vanish. Then $F_2(Fl_1, Fl_2) \neq 0$ by assumption. We compute the fifth partial wave invariant. Again all cases of the form $l[0, \dots]$ are unsupported. Additionally, cases must not contain any sums. For example, $l[c_1, c_2, -c_1 - c_2]_Q = \emptyset$, because the condition $Fl_1(l_2) \neq 0$ implies that l_1 and l_2 are not proportional. This leaves the three cases $l[c_1, -c_1]$, $l[c_1, -c_1, c_1, -c_1]$ and $l[c_1, c_2, -c_2, -c_1]$ as the only supported cases. The Q-sums of the latter two cases can be shown to cancel each other. In the Q-sum of $l[c_1, -c_1]$ all terms except the one containing $\tilde{F}_2$ vanish and it thus evaluates to

$$\mathsf{wi}_{5,l}(Q) = Q_{-Fl_1} Q_{-Fl_2} \frac{960}{Fl_1(l)^4} \cdot F_2(Fl_1, Fl_2)\,.$$

Similarly,

$$\mathsf{wi}_{5,-l}(Q) = Q_{Fl_1} Q_{Fl_2} \frac{960}{Fl_1(l)^4} \cdot F_2(Fl_1, Fl_2)\,.$$

Details can be found in the MATHEMATICA notebook in Appendix D. Since $F_2(Fl_1, Fl_2) \neq 0$ we can again conclude that (Q, a, b) must be of the same type with respect to both Fl_1 and Fl_2. □

Let us now find examples where the preceding Lemma 6.12 can be applied.

Remark 6.13 (Nondegeneracy).
A lattice $\mathcal{L}$ is nondegenerate exactly if there are no two nontrivial lattice vectors that are orthogonal. If $l_1, l_2 \in \mathcal{L}\backslash\{0\}$ are orthogonal then $l_1 + l_2$ and $\pm(l_1 - l_2)$ are distinct but $|l_1 + l_2| = |l_1 - l_2|$. If, conversely, $|l_1| = |l_2|$ and $l_1 \neq \pm l_2$ then

$$\langle l_1 + l_2, l_1 - l_2 \rangle = |l_1|^2 - |l_2|^2 = 0 \qquad \text{and} \qquad l_1 + l_2 \neq 0 \neq l_1 - l_2\,.$$

Example 6.14 (Dimension 2).
When is a lattice $\mathcal{L}$ of dimension 2 nondegenerate? Without loss of generality we assume that a lattice basis (U_1, V_1) for $\mathcal{L}$ is given by the columns of the matrix (in standard coordinates)

$$B = \begin{pmatrix} 1 & x \\ 0 & y \end{pmatrix} \qquad \text{with} \qquad B^{-T} = \begin{pmatrix} 1 & 0 \\ -x/y & 1/y \end{pmatrix}.$$

Here, $B^{-T} \coloneqq (B^{-1})^T$. The columns of B^{-T} are, in standard dual coordinates, basis vectors (U^1, V^1) for the dual lattice $\mathcal{L}'$.

For arbitrary integers $\alpha, \beta, a, b \in \mathbb{Z}$ we have

$$\langle \alpha U_1 + \beta V_1, a U_1 + b V_1 \rangle = (\alpha + \beta x)(a + bx) + \beta b y^2$$

and

$$\begin{aligned} \langle \beta U^1 - \alpha V^1, b U^1 - a V^1 \rangle &= \beta b + (\beta x/y + \alpha/y)(bx/y + a/y) \\ &= \frac{1}{y^2}\Big((\alpha + \beta x)(a + bx) + \beta b y^2\Big). \end{aligned}$$

It follows that there are nontrivial but orthogonal lattice vectors in $\mathcal{L}$ exactly if there are such vectors in $\mathcal{L}'$. Thus, $\mathcal{L}$ is nondegenerate exactly if $\mathcal{L}'$ is nondegenerate.

If we choose two lattice vectors $l_1, l_2 \in \mathcal{L}$ with $Fl_1(l_2) \neq 0$ (or equivalently in dimension 2: $\{l_1, l_2\}$ linearly independent) then $l_1 \neq 0 \neq l_2$ and thus $Fl_1 \neq 0 \neq Fl_2$. If the lattice $\mathcal{L}$ is nondegenerate and of dimension 2 then $\mathcal{L}'$ is nondegenerate and $F_0(Fl_1, Fl_2) = \langle Fl_1, Fl_2 \rangle \neq 0$. Let Q be a potential with frequency support $\{\pm Fl_1, \pm Fl_2\}$. Lemma 6.12 implies that two connections a and b are isospectral with respect to Q if and only if (Q, a, b) is of type (M) or of type (P).

The previous example only holds in dimension 2. In larger dimensions there are nondegenerate lattices with degenerate dual lattices.

Example 6.15. Consider a four-dimensional lattice $\mathcal{L}$ with a lattice basis given by the following matrix:

$$B = (U_1, U_2, V_1, V_2) = \begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ 0 & x_4 & 0 & 0 \\ 0 & 0 & x_5 & 0 \\ 0 & 0 & 0 & x_6 \end{pmatrix} \qquad \text{with } x_1, \dots, x_6 \neq 0.$$

We choose each x_i such that x_i and x_i^2 are rationally independent of the x_j, $j < i$, and their products (with $x_0 = 1$). Then $\mathcal{L}$ is nondegenerate. Again, the dual basis is given by

$$B^{-T} = (U^1, U^2, V^1, V^2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -x_1/x_4 & 1/x_4 & 0 & 0 \\ -x_2/x_5 & 0 & 1/x_5 & 0 \\ -x_3/x_6 & 0 & 0 & 1/x_6 \end{pmatrix}$$

and obviously three of those dual basis vectors are orthogonal. Thus, $\mathcal{L}'$ is degenerate. In this example we can choose $l_1 \coloneqq U_2$ and $l_2 \coloneqq V_2$, which implies that

$$Fl_1(l_2) = F(U_2, V_2) = r_2 \neq 0 \qquad \text{but} \qquad Fl_1 = r_2 V^2 \perp -r_2 U^2 = Fl_2$$

hence $F_0(Fl_1, Fl_2) = 0$.

However, it is not difficult to show that

$$F_1(Fl_1, Fl_2) = \frac{r_2^3}{x_4^2 x_6^2} \neq 0\,.$$

We can again apply Lemma 6.12 to obtain that for a potential Q with frequency support $\{\pm FU_2, \pm FV_2\}$ two connections a and b are isospectral if and only if (Q, a, b) is of type (M) or of type (P).

Let us consider one further example, which actually uses the part of Lemma 6.12 that relies on the fifth wave invariant, that is, where we have the situation $0 = F_0(Fl_1, Fl_2) = F_1(Fl_1, Fl_2)$ but $F_2(Fl_1, Fl_2) \neq 0$.

Example 6.16 (Using the fifth wave invariant).
We again consider a four lattice $\mathcal{L}$ with lattice basis given by the matrix

$$B = (U_1, U_2, V_1, V_2) = \begin{pmatrix} 1 & 0 & 0 & x_1 \\ 0 & 0 & 0 & x_2 \\ 0 & x_3 & 0 & 0 \\ 0 & x_4 & x_5 & x_6 \end{pmatrix} \quad \text{with} \quad B^{-T} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -\frac{x_1}{x_2} & 0 & \frac{-x_6}{x_2 x_5} & \frac{1}{x_2} \\ 0 & \frac{1}{x_3} & \frac{-x_4}{x_3 x_5} & 0 \\ 0 & 0 & \frac{1}{x_5} & 0 \end{pmatrix}.$$

The determinant of B is $x_2x_3x_5$, which must be nonzero; so we require $x_2, x_3, x_5 \neq 0$. U_1 is orthogonal to U_2 and V_1 and thus $\mathcal{L}$ is degenerate. But if we again chose $l_1 \coloneqq U_2$ and $l_2 \coloneqq V_2$ then Lemma 6.12 may be applied if there are only two lattice vectors of length $|l_1 + l_2|$ in $\mathbb{Z}(l_1, l_2)$.

For $\alpha, \beta \in \mathbb{Z}$

$$|\alpha l_1 + \beta l_2|^2 = \beta^2 x_1^2 + \beta^2 x_2^2 + \alpha^2 x_3^2 + (\alpha x_4 + \beta x_6)^2 .$$

We now assume that all x_2, x_3, x_4 and x_6 are rational but that x_1^2 is irrational. Hence, if $|\alpha l_1 + \beta l_2| = |l_1 + l_2|$ then $\beta^2 = 1$. Without loss of generality we may assume that $\beta > 0$ (otherwise we continue this calculation with $-\alpha$ and $-\beta$). Thus, $\beta = 1$ and

$$\begin{aligned} 0 = |\alpha l_1 + \beta l_2|^2 - |l_1 + l_2|^2 &= (\alpha^2 - 1)x_3^2 + (\alpha x_4 + x_6)^2 - (x_4 + x_6)^2 \\ = (\alpha^2 - 1)x_3^2 + (\alpha^2 - 1)x_4^2 + 2(\alpha - 1)x_4x_6 &= (\alpha^2 - 1)(x_3^2 + x_4^2) + 2(\alpha - 1)x_4x_6 \\ &= (\alpha - 1) \cdot \Big((\alpha + 1)(x_3^2 + x_4^2) + 2x_4x_6\Big). \end{aligned}$$

If we assume that $2x_4x_6/(x_3^2 + x_4^2) \notin \mathbb{Z}$ it follows that $\alpha = \beta = 1$ and that $|\alpha l_1 + \beta l_2| = |l_1 + l_2|$ implies $\alpha = \beta = 1$ or $\alpha = \beta = -1$.

Further, we still need that $|l_1| = x_3^2 + x_4^2 \neq |l_2| = x_1^2 + x_2^2 + x_6^2$. But this inequation already follows from the assumption that x_1^2 is irrational but the other four squares are not.

Finally, we need to compute $F_i(Fl_1, Fl_2)$ for $i = 0, 1, 2$ given our choices. It is not hard to show that

$$F_0(Fl_1, Fl_2) = 0 .$$

Further, we have that

$$F_1(Fl_1, Fl_2) = \frac{r_2^2(x_5r_2 - x_1x_4r_1)}{x_2^2x_3^2x_5} .$$

We have not made any assumption regarding x_5 other than that it must be nonzero. So, letting

$$x_5 \coloneqq \frac{r_1x_1x_4}{r_2} ,$$

we have

$$F_1(Fl_1, Fl_2) = 0 .$$

Finally, a tedious calculation (or a small MATHEMATICA notebook) gives us

$$F_2(Fl_1, Fl_2) = \frac{x_4x_6r_1^2r_2^2}{x_2^2x_3^2x_5^2} \neq 0$$

by the assumption above. Therefore, the fifth wave invariant gives us via Lemma 6.12 that the two connections a and b are isospectral with respect to a potential Q with frequency support $\{\pm Fl_1, \pm Fl_2\}$ on the lattice described above with $l_1 = U_2$ and $l_2 = V_2$ if and only if (Q, a, b) is of type (M) or of type (P).

A concrete lattice that satisfies all the above conditions would be given, for example, by the lattice basis matrix

$$\begin{pmatrix} 1 & 0 & 0 & \sqrt[4]{2} \\ 0 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 1 & \frac{r_1}{r_2}\sqrt[4]{2} & 1 \end{pmatrix}.$$

6.2 Degenerate Case

The second partial small wave invariant of Theorem 5.8 is

$$\mathsf{wi}_{2,l}(Q) = Q_{-Fl}\frac{|\tilde{Fl}|^2}{6} + \sum_{c \in l[0,0]}^{Q} 1\,.$$

If the lattice support $\mathcal{L}_Q$ is nondegenerate or if the torus M is two dimensional then we can drop the first summand of this invariant by Theorem 5.13 and still obtain a spectral invariant

$$\mathsf{wi}^{s}_{2,l}(Q) = \sum_{c \in l[0,0]}^{Q} 1\,.$$

In this section we will consider an example where those assumptions are not satisfied and Theorem 5.13 does not apply. In fact, $\mathsf{wi}^{s}_{2,l}(Q)$ vanishes in this example and we will use the first summand of $\mathsf{wi}_{2,l}(Q)$ together with $\mathsf{wi}_{1,l}(Q)$ to show that two translation-invariant connections are isospectral exactly if they are of mixed type with respect to the chosen potential Q.

This example is closely related to Example 5.11.

It follows that the first term of the second partial wave invariant $\mathsf{wi}_{2,l}(Q)$ can carry information beyond those contained within $\mathsf{wi}_{1,l}(Q)$ and $\mathsf{wi}^{s}_{2,l}(Q)$. Furthermore, in the proof of Lemma 6.7 we have used that the second term of this partial wave invariant does not vanish. Therefore, this sum is a minimal expression for the second partial wave invariant and cannot be simplified further without additional assumptions.

Example 6.17. Consider a four dimensional lattice $\mathcal{L}$ for which the Chern lattice basis is given by

$$U_1 \coloneqq e_1\,, \quad U_2 \coloneqq e_2\,, \quad V_1 \coloneqq e_3\,, \quad V_2 \coloneqq \alpha \cdot e_4 \qquad \text{with } \alpha > 0.$$

We choose a potential Q with frequencies on the lattice with the lattice support

$$\mathcal{L}_Q := \{\pm U_1, \pm U_2\}\,.$$

Note that $\mathcal{L}_Q$ is degenerate: $|\pm U_1| = 1 = |\pm U_2|$. The only nontrivial first small wave invariant is found at $d = 1$:

$$\begin{aligned}\mathsf{wi}_{1,1}(a,Q) &= E_a(U_1)Q_{-FU_1} + E_a(-U_1)Q_{FU_1} \\ &\quad + E_a(U_2)Q_{-FU_2} + E_a(-U_2)Q_{FU_2}\,,\end{aligned}$$

because $\sigma_l = 1$ for all $l \in \mathcal{L}_Q$. The degeneracy of the lattice support causes this wave invariant to have more than two summands. In contrast to the proof of Lemma 6.2 we cannot conclude from the first wave invariant alone that isospectrality of a and b with respect Q implies that (Q, a, b) are of mixed type.

However, we have

$$l[0,0]_Q = \emptyset \qquad \text{for all } l \in \mathcal{L}_Q,$$

because no sum of two elements of $F\mathcal{L}_Q$ can be equal to $-Fl$. Thus, the nontrivial second small partial wave invariants are

$$\mathsf{wi}_{2,l}(Q) = Q_{-Fl}\frac{|\tilde{F}l|^2}{6} + \sum_{c\in l[0,0]}^{Q} 1 = Q_{-Fl}\frac{|\tilde{F}l|^2}{6}\,.$$

We have

$$|\pm FU_1| = |r_1 V^1| = r_1 \qquad \text{and} \qquad |\pm FU_2| = |r_2 V^2| = \frac{r_2}{\alpha}|e^4| = \frac{r_2}{\alpha}\,.$$

The second wave invariant with respect to length 1 is thus given by

$$\begin{aligned}\frac{6}{4\pi^2}\mathsf{wi}_{2,1}(a,Q) &= r_1^2\Big(E_a(U_1)Q_{-FU_1} + E_a(-U_1)Q_{FU_1}\Big) \\ &\quad + \frac{r_2^2}{\alpha^2}\Big(E_a(U_2)Q_{-FU_2} + E_a(-U_2)Q_{FU_2}\Big)\,.\end{aligned}$$

If we choose the Chern invariant factors $r_1|r_2$ and α such that $r_1 \neq r_2/\alpha$ then

$$\mathsf{wi}_{1,1}(a,Q) - \frac{6}{(2\pi r_1)^2}\mathsf{wi}_{2,1}(a,Q) = (1 - (\frac{r_2}{\alpha r_1})^2)\Big(E_a(U_2)Q_{-FU_2} + E_a(-U_2)Q_{FU_2}\Big)$$

is a nonzero spectral invariant, and hence, so is

$$E_a(U_1)Q_{-FU_1} + E_a(-U_1)Q_{FU_1}\,.$$

As in the proof of Lemma 6.2 it now follows by Lemma 6.1 that that (Q, a, b) must be of mixed type if a and b are isospectral with respect to Q.

One might now be tempted to use higher invariants on lattice vectors like $U_1 + U_2$ to again obtain a link between the types of (Q, a, b) with respect to FU_1 and FU_2. Since $Q_{-Fl} = 0$ for $|l| = \sqrt{2}$, a computation shows that

$$\begin{aligned}\mathsf{wi}_{2,\sqrt{2}}(a, Q) &= 4\operatorname{Re}\Big(E_a(U_1 + U_2)Q_{-FU_1}Q_{-FU_2} + E_a(U_1 - U_2)Q_{-FU_1}Q_{FU_2}\Big) \\ &= 8\operatorname{Re}\Big(E_a(U_1)Q_{-FU_1}\Big) \cdot \operatorname{Re}\Big(E_a(U_2)Q_{-FU_2}\Big).\end{aligned}$$

If (Q, a, b) is of type (M) or of type (P) with respect to U_i, then

$$\operatorname{Re}\Big(E_a(U_i)Q_{-FU_i}\Big) = \operatorname{Re}\Big(E_b(U_i)Q_{-FU_i}\Big)$$

by Lemma 6.1. So in that case we do indeed have $\mathsf{wi}_{2,\sqrt{2}}(a, Q) = \mathsf{wi}_{2,\sqrt{2}}(b, Q)$ but the two lattice vectors U_1 and U_2 are decoupled and this wave invariant does not provide any additional information.

For comparison, the second simple wave invariant used in the proof of Lemma 6.7 did not decouple. In the setting of Lemma 6.7 and with $l = l_i + l_{i+1}$ we had

$$\begin{aligned}\mathsf{wi}^{\mathrm{s}}_{2,|l|}(a, Q) &= 2\sigma_l\Big(E_a(l)Q_{-Fl_i}Q_{-Fl_{i+1}} + E_a(-l)Q_{Fl_i}Q_{Fl_{i+1}}\Big) \\ &= 4\sigma_l \operatorname{Re}\Big(E_a(l_i)Q_{-Fl_i} \cdot E_a(l_{i+1})Q_{-Fl_{i+1}}\Big).\end{aligned}$$

A subtle but important difference.

A similar effect occurs for the third wave invariant $\mathsf{wi}_{3,\sqrt{5}}(a, Q)$. This invariant also contains products of U_1- and U_2-terms that decouple. So again we do not obtain any information beyond (Q, a, b) being of mixed type.

Indeed, it is to be expected that this can happen since by Lemma 2.17 the two connections a and b are already isospectral if (Q, a, b) is of mixed type.

Therefore, we have in this example that a and b are isospectral with respect to Q if and only if (Q, a, b) is of mixed type.

6.3 Vanishing Wave Invariants

So far we have used the first five wave invariants to study special potentials and their implications on the isospectrality of translation-invariant connections. In this section we will ask more generally: Which potentials Q have the property that *not* all translation-invariant connections are isospectral with respect to Q?

By Corollary 2.15 all translation-invariant connections are isospectral for constant potentials. On the other hand, we have shown in Corollary 4.39 that if all translation-invariant connections are isospectral then all partial wave invariants must vanish.

Thus, we ask: Are there nonvanishing partial wave invariants for a given nonconstant potential?

Conjecture 6.18. Given any flat torus $M = \mathbb{R}^n/\mathcal{L}$ with a Chern basis and some Chern invariant factors and a smooth real-valued nonconstant potential $Q \in C^\infty(M)$ then there is exists a $k \in \mathbb{N}$ and a a lattice vector $l \in \mathcal{L}\backslash\{0\}$ such that the k-th partial wave invariant is not zero:

$$\mathsf{WI}_{k,l}(Q) \neq 0 \qquad \text{for all } a \in \mathbb{R}^{n\prime}.$$

Consequently, by Corollary 4.39, there exist nonisospectral translation-invariant connections for every nonconstant potential.

This conjecture is trivially true if the Chern invariant factors are all 1:

Lemma 6.19. If the largest Chern invariant factor r_m is one then for every nonconstant smooth real-valued potential Q there exist nonisospectral translation-invariant connections.

Proof. If $r_m = 1$ then all Chern invariant factors are one and $F\colon \mathcal{L} \to \mathcal{L}'$ is bijective. If Q is nonconstant there exists a $c \in \mathcal{L}'\backslash\{0\}$ such that $Q_c \neq 0$. Letting $l \in \mathcal{L}$ be such that $c = -Fl$, we obtain

$$\mathsf{wi}_{1,l}(Q) = Q_{-Fl} \neq 0\,. \qquad \square$$

If the Chern invariant factors are not all 1 and thus F not surjective then the situation is more complicated. We start with a theorem that gives limits, for any $K \in \mathbb{N}$, of the information that the first K wave invariants can provide.

Theorem 6.20. Let M denote any flat, even-dimensional torus. Given any $K \in \mathbb{N}$ we can choose Chern invariant factors and a nonconstant potential Q such that the first K partial wave invariants vanish for every lattice vector $l \in |\mathcal{L}|\backslash\{0\}$:

$$\mathsf{WI}_{k,l}(Q) = 0 \qquad \text{for all } k \leq K.$$

In particular, for all translation-invariant connections $a, b \in \mathbb{R}^{n\prime}$

$$\mathsf{WI}_{k,d}(a, Q) = 0 = \mathsf{WI}_{k,d}(b, Q) \qquad \text{for all } k \leq K.$$

In fact, it will suffice to choose the Chern invariant factors such that $r_1 > K$. Given Chern invariant factors with $r_1 > K$ we can find two nonisospectral potentials Q and P such that the first K wave invariants are equal and even zero:

$$\mathsf{WI}_{k,d}(a, Q) = 0 = \mathsf{WI}_{k,d}(a, P) \qquad \text{for all } k \leq K \text{ and } a \in \mathbb{R}^{n\prime}.$$

Proof. By Theorem 4.42 the wave invariants are of the form

$$\mathsf{WI}_{k,d}(a,Q) = \sum_{|l|=d} E_a(l)\sigma_l \sum_{s\in\mathcal{S}_k} \langle C_s(Q), E_{-Fl}\rangle\,,$$

where the $C_s(Q)$ are polynomials in Q that depend on x only via the potential Q. By Lemma B.4 those polynomials are always of the form

$$C\cdot Q(x+\tau^{b_1}l,d_1)\cdots Q(x+\tau^{b_q},d_q) \qquad \text{(confer Definition 4.45)}$$

and the order q of Q in these terms is less than or equal to k. Choose as the first Chern invariant factor any integer $r_1 > K$. Since $r_1 | \cdots | r_m$ the other Chern invariant factors are also larger than K. If $\{U_i, V_i\}$ is the Chern basis of $\mathcal{L}$ and $\{U^i, V^i\}$ the corresponding dual basis of $\mathcal{L}'$ choose a potential Q with $\mathcal{L}'_Q \subset \{\pm U^i, \pm V^i\}$.

Let $i \in \{1,\dots,n/2\}$. If $k \le K$ and $l \in \mathcal{L}\backslash\{0\}$ is a nonzero lattice vector with $V^i(l) \neq 0$ then for such a choice of Chern invariant factors and potential we have for $c \in (\mathcal{L}'_Q)^q$, writing $\sum c := c_1 + \cdots + c_q$, that $c_h(U_i) \in \{-1,0,1\}$ for all $h \in \{1,\dots,q\}$ and thus

$$|(\Sigma c + Fl)(U_i)| \ge |Fl(U_i)| - |\Sigma c(U_i)| \ge r_i|V^i(l)| - q \ge r_1 - k \ge r_1 - K > 0\,.$$

If on the other hand $U^i(l) \neq 0$ then

$$|(\Sigma c + Fl)(V_i)| \ge |Fl(V_i)| - |\Sigma c(V_i)| \ge r_i|U^i(l)| - q) \ge r_1 - k \ge r_1 - K > 0\,.$$

Either way, we always have for all multiindices $c \in (\mathcal{L}'_Q)^q$ that

$$c_1 + \cdots + c_q + Fl \neq 0\,.$$

This implies $\langle C_s(Q), E_{-Fl}\rangle = 0$. Therefore, for all $l \in \mathcal{L}\backslash\{0\}$

$$\mathsf{WI}_{k,l}(Q) = 0 \qquad \text{and hence} \qquad \mathsf{WI}_{k,d}(a,Q) = 0$$

for all $a \in \mathbb{R}^{n\prime}$ and all $d \in |\mathcal{L}|\backslash\{0\}$.

By the heat invariants given in Theorem 3.28 the L^2-norm of the potential is spectrally determined. If we choose two potentials P and Q as above but such that

$$\|P\|_{L^2} \neq \|Q\|_{L^2}$$

they are nonisospectral but have the same first K wave invariants, which are, in fact, zero. □

Remark 6.21. Note that the proof of Theorem 6.20 shows that there are infinitely many choices of Chern invariants and potentials with the properties required in Theorem 6.20. The Chern invariants need only be large and the potentials need to have vanishing Fourier coefficients for "high frequencies".

6.4 Extremal Frequencies

We have shown in the previous section that the first wave invariants may vanish if the Chern invariants are large but the supported frequencies are small. On the other hand, we will now show that if the frequency support has *extremal frequencies* then there is always some nonvanishing partial wave invariant $\mathsf{WI}_{k,l}(Q)$, even if its index k may need to be very large.

Definition 6.22. For any basis B of $\mathbb{R}^n$ with $B \subset \mathcal{L}$ denote by B_i the i-th basis vector in B and set $B_{-i} = B_i$. A tuple $I = (i_1, \dots, i_k) \in \{\pm 1, \dots, \pm n\}^k$ is said to give *directions* if $\#\{|i_1|, \dots, |i_k|\} = k$. Given some directions I introduce the following sets for any $\mathcal{M} \subset \mathcal{L}'$:

$$\mathcal{M}(B,(i)) \coloneqq \left\{ c \in \mathcal{M} \mid c(B_i) = \sup_{d \in \mathcal{M}} d(B_i) \right\} \qquad \text{for } i > 0 \text{ and}$$
$$\mathcal{M}(B,(i)) \coloneqq \left\{ c \in \mathcal{M} \mid c(B_i) = \inf_{d \in \mathcal{M}} d(B_i) \right\} \qquad \text{for } i < 0.$$

For tuples of length greater than 1 set

$$\mathcal{M}(B,(i_1,\dots,i_k)) \coloneqq (\mathcal{M}(B,(i_1,\dots,i_{k-1}))(B,(i_k)) .$$

In other words, the set $\mathcal{M}(B,I)$ is constructed from $\mathcal{M}$ by repeatedly selecting the maximal or minimal elements of $\mathcal{M}$ in the directions given by I with respect to the basis B. Of course, this set may be empty if one of the appearing sets is not bounded in the direction under consideration.

Definition 6.23 (Extremal Frequency).
A smooth real-valued nonconstant potential $Q \in C^\infty(M)$ has an *extremal frequency* $c^* \in \mathcal{L}'$ if there exists a basis B of $\mathbb{R}^n$ and some directions I such that

$$\mathcal{L}'_Q(B,I) = \{c^*\} .$$

Recall that $m = n/2$.

Theorem 6.24. For every nonconstant potential $Q \in C^\infty(M)$ with an extremal frequency there exists a lattice vector $l \in \mathcal{L}\backslash\{0\}$ such that the partial wave invariant $\mathsf{WI}_{r_m,l}(Q)$ is nonzero. In particular, by Corollary 4.39 there exist translation-invariant connections which are nonisospectral with respect to Q.

Proof. Let $c^* \in \mathcal{L}'$ be an extremal frequency with respect to the basis B with directions I. With the inverse $G\colon \mathbb{R}^{n\prime} \to \mathbb{R}^n$ of the map $F\colon \mathbb{R}^n \to \mathbb{R}^{n\prime}$ we have

$$Gc^* = G\sum_{i=1}^{m}\big(c^*(U_i)U^i + c^*(V_i)V^i\big) = \sum_{i=1}^{m}\big(-\frac{c^*(U_i)}{r_i}V_i + \frac{c^*(V_i)}{r_i}U_i\big).$$

This vector Gc^* is not necessarily a lattice vector but because $r_1 | \cdots | r_m$ the multiple $r_m Gc^* \in \mathcal{L}$ is. Set

$$l := -r_m Gc^* \in \mathcal{L}\,.$$

Conversely, we have $-Fl = -F(-r_m Gc^*) = r_m c^*$.

In the following we show that $\mathsf{WI}_{r_m,l}(Q) \neq 0$. By Theorem 4.42 the partial wave invariant is of the form

$$\mathsf{WI}_{r_m,l}(Q) = \sum_{s \in S'_{r_m}} \langle C_s(Q), E_{-Fl} \rangle \qquad \text{for all } r_m \in \mathbb{N},$$

where each $C_s(Q)$ is a monomial in Q that has no dependency on $x \in M$ other than through the potential Q. It follows that for such summands to be nonzero, $\langle C_s(Q), E_{-Fl} \rangle \neq 0$, it is necessary that

$$\exists_{c \in (\mathcal{L}'_Q)^k} : \Sigma\, c = -Fl = r_m c^*\,,$$

where k is the order of Q in $C_s(Q)$.

Because $c \in \mathcal{L}'_Q$ implies $-c \in \mathcal{L}'_Q$ we have that if $c^*(B_{I_1}) = 0$ then all elements of $\mathcal{L}'_Q$ vanish in B_{I_1}-direction and are thus both maximal and minimal in this direction. Thus, $c^*(B_{I_1}) = 0$ implies $\mathcal{L}'_Q(B,(I_1)) = \mathcal{L}'_Q$. Since Q is nonconstant we have $\mathcal{L}'_Q \neq \{0\}$ and we may assume that $c^*(B_{I_1}) \neq 0$ without loss of generality.

Consider first the case that $I_1 > 0$, which means that c^* is maximal in B_{I_1}-direction. Then, for all $c \in (\mathcal{L}'_Q)^k$

$$\Sigma\, c(B_{I_1}) \leq k c^*(B_{I_1}),$$

so the lowest order k of Q in $C_s(Q)$ for which $\langle C_s(Q), E_{-Fl} \rangle = \langle C_s(Q), E_{\Sigma\, c} \rangle$ can be nonzero is $k = r_m$. Additionally, $\Sigma\, c(B_{I_1}) = r_m c^*(B_{I_1})$ for some $c \in (\mathcal{L}'_Q)^{r_m}$ implies $c_i \in \mathcal{L}'_Q(B,(I_1))$ for all $i = 1, \ldots, r_m$.

On the other hand, if $I_1 < 0$ and c^* is minimal in B_{I_1}-direction then

$$\Sigma\, c(B_{I_1}) \geq k c^*(B_{I_1}) \qquad \text{for all } c \in (\mathcal{L}'_Q)^k.$$

Since $c \in \mathcal{L}'_Q$ implies $-c \in \mathcal{L}'_Q$ and since we have assumed that $c^*(B_{I_1}) \neq 0$ we must have $c^*(B_{I_1}) < 0$. Again, any monomial $C_s(Q)$ with $\langle C_s(Q), E_{-Fl} \rangle \neq 0$ must have order $k = r_m$ or greater, and $\Sigma\, c(B_{I_1}) = r_m c^*(B_{I_1})$ implies $c_i \in \mathcal{L}'_Q(B,(I_1))$ for all $i = 1, \ldots, r_m$.

In fact, we can apply the same reasoning inductively:

$$\Sigma\, c(B_{I_s}) = r_m c^*(B_{I_s}) \qquad \text{implies} \qquad c_i \in \mathcal{L}'_Q(B,(I_1,\ldots,I_s))$$

for all $i = 1 \ldots, r_m$ and $s \le |I|$. In particular, if $c \in l[0,\ldots,0]_Q$ has length r_m then $c_i \in \mathcal{L}'_Q(B,(I_1,\ldots,I_{|I|})) = \mathcal{L}'_Q(B,I) = \{c^*\}$. Moreover, $c^*(l) = -\frac{1}{r_m} Fl(l) = 0$ and therefore we have

$$l[0,\ldots,0]_Q = \{(c^*,\ldots,c^*)\} \qquad \text{in } (\mathcal{L}'_Q)^{r_m}.$$

Since $\langle C_s(Q), E_{-Fl}\rangle = 0$ if $C_s(Q)$ has order $k < r_m$ in Q, it follows from Lemma B.36 that that $\mathsf{WI}_{k,l}(Q) = 0$ for all $k < r_m$. Additionally, all terms except the highest Q-order term in $\mathsf{WI}_{r_m,l}(Q)$, that is, the term of order r_m, vanish. By Lemma B.36

$$\mathsf{WI}_{r_m,l}(Q) = \Big(\frac{\mathrm{i}}{2}|l|\Big)^{r_m} \sum_{c\in l[0,\ldots,0]}^{Q} \frac{1}{r_m!} = \Big(\frac{\mathrm{i}}{2}|l|\Big)^{r_m} Q^{r_m}_{c^*} \frac{1}{r_m!} \neq 0\,.$$

□

Example 6.25. If the frequency support $\mathcal{L}'_Q$ of the potential Q is finite then Q has extremal frequencies, Theorem 6.24 applies and there must exist non-isospectral connections.

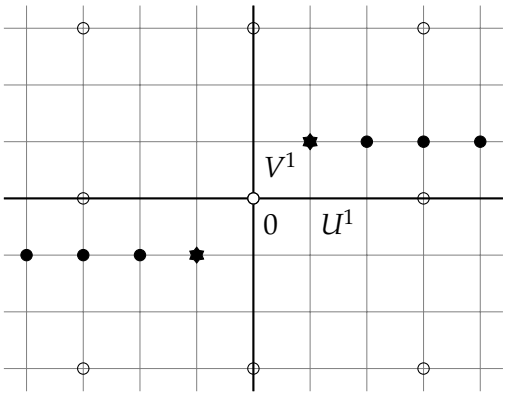
Example 6.26. Consider the case of $r_1 = 3$ and some potential Q with frequency support contained in the solid points of figure 6.2,

$$\mathcal{L}'_Q \subset \left\{\pm(kU^1 + V^1) \mid k \in \mathbb{N}\right\}.$$

Figure 6.2: The component of $\mathcal{L}'$ corresponding to U^1 and V^1. Solid points give the frequency support of Q and empty ones $F\mathcal{L}$,

$$FU_1 = 3V^1 \quad \text{and} \quad FV_1 = -3U^1\,.$$

Extremal frequencies are marked by stars.



Assuming that $Q_{U^1+V^1} \neq 0$ we have with $B = \{U_1, V_1, \ldots\}$ that

$$\mathcal{L}'_Q(B,(2,-1)) = \{U^1 + V^1\}\,.$$

The potential has extremal frequencies, and Theorem 6.24 applies: There must be nonisospectral connections.

Similarly, if $\mathcal{L}'_Q \subset \left\{\pm((k+1)U^1 + kV^1) \mid k \in \mathbb{N}\right\}$ with $Q_{2U^1+V^1} \neq 0$, see figure 6.3, then a basis $B = \{-U_1 + V_1, V_1, \ldots\}$ gives

$$\mathcal{L}'_Q(B,(1)) = \left\{-((k+1)U^1 + kV^1) \mid k \in \mathbb{N}\right\},$$

because $-((k+1)U^1 + kV^1)(-U_1 + V_1) = (k+1) - k = 1 > -1 = ((k+1)U^1 + kV^1)(-U_1 + V_1)$. Hence,

$$\mathcal{L}'_Q(B, (1,2)) = \{-2U^1 - V^1\}.$$

Again, Theorem 6.24 applies and there must exist nonisospectral connections.

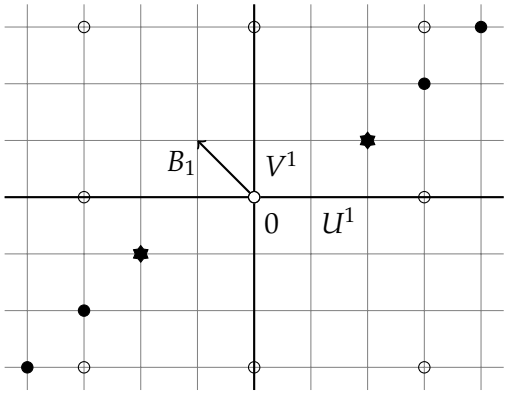


Figure 6.3: Frequency support $\mathcal{L}'_Q = \{\pm((k+1)U^1 + kV^1)\}$ with extremal frequencies.

Example 6.27. On the other hand there are also potentials that have a frequency support that is bounded in some directions but there exists no basis B and tuple I as in Theorem 6.24. Take for example

$$\mathcal{L}'_Q = \left\{\pm kU^1 \pm V^1 \mid k \in \mathbb{N}\right\}$$

given in figure 6.4.

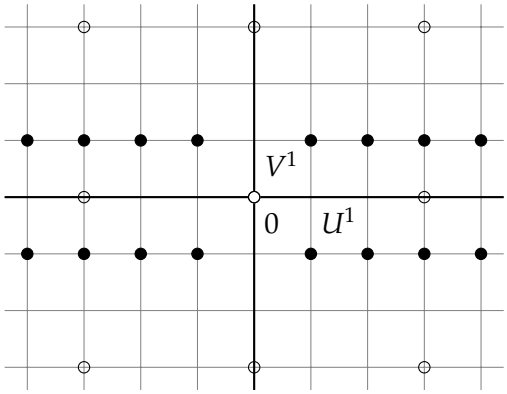


Figure 6.4: Frequency support without extremal frequencies.

For the proof of Theorem 6.29 below we need the following notion of one-dimensional potentials.

Definition 6.28. Given a smooth, real-valued potential Q on M and a nonzero dual lattice vector $c \in \mathcal{L}' \backslash \{0\}$ we say that

$$Q^c := \sum_{d \in \mathcal{L}' \cap \mathbb{R}c \backslash \{0\}} Q_d E_d$$

is the one-dimensional potential in the direction c given by Q.

The one-dimensional potentials differ from Q in that some Fourier coefficients are set to zero. Since the smoothness of Q and Q^c depends on their Fourier coefficients going to zero sufficiently fast Q^c is again smooth. We also still have that $(Q^c)_{-d} = \overline{(Q^c)_d}$ and thus that Q^c is real-valued.

Theorem 6.29. If the torus M is two-dimensional and if the only Chern invariant factor $r := r_1$ is smaller than three,

$$r \in \{1, 2\},$$

then for every nonconstant smooth real-valued potential Q there exist non-isospectral translation-invariant connections.

Proof. The case that $r = 1$ has already been proven in Lemma 6.19. Assume $r = 2$. Then $F \colon \mathcal{L} \to \mathcal{L}'$ is only injective but not surjective. Should there exist a $c^* \in \mathcal{L}'_Q \backslash \{0\}$ such that $Gc \in \mathbb{R}^n$ happens to be a (nonzero) lattice vector, $Gc \in \mathcal{L}$, then it follows that $\mathsf{wi}_{1,Gc}(Q) \neq 0$ as in the proof of Lemma 6.19 and there must be nonisospectral connections by Corollary 4.39.

It remains to show the claim for the case that $r = 2$ and that $\mathcal{L}'_Q \cap F\mathcal{L} \backslash \{0\} = \emptyset$. Since M is two-dimensional this implies that $c(U_1)$ or $c(V_1)$ are odd for all $c \in \mathcal{L}'_Q \backslash \{0\}$.

Since Q is nonconstant there exists a $c^* \in \mathcal{L}'_Q \backslash \{0\}$ and for such a c^* we can find a nonzero lattice vector $l^* = l^*_1 U_1 + l^*_2 V_1 := -c^*(U_1)V_1 + c^*(V_1)U_1 \in \mathcal{L}$ with $c^*(l^*) = 0$. For this choice of l^* we also have that l^*_1 or l^*_2 are odd.

We consider the one-dimensional potential Q^{c^*} in the direction of c^* given by Q. Per definitionem the frequency support of this one-dimensional potential is contained in $\mathbb{R}c^*$ and so is the frequency support of its square, $(Q^{c^*})^2$. We now show that additionally

$$\langle (Q^{c^*})^2, E_c \rangle \neq 0 \qquad \text{implies} \qquad c \in F\mathcal{L}.$$

Given two c_1 and c_2 in the frequency support of Q^{c^*} we have

$$0 = c_i(l^*) = c_i(U_1) l^*_1 + c_i(V_1) l^*_2 .$$

If both l^*_1 and l^*_2 are odd then $c_i(U_1)$ is even if and only if $c_i(V_1)$ is even. Because $c_i \notin F\mathcal{L}$ at least one of those integers must be odd. Therefore, $c_i(U_1)$ and $c_i(V_1)$

are both odd for $i = 1$ and $i = 2$. Thus, $(c_1 + c_2)(U_1)$ and $(c_1 + c_2)(V_1)$ are both even, hence $c_1 + c_2 \in F\mathcal{L}$.

If only, say, l_1^* is odd and l_2^* is even then $c_i(U_1)$ must be even and therefore $c_i(V_1)$ must be odd for $i = 1, 2$. Again, $c_1 + c_2 \in F\mathcal{L}$.

Further, $(Q^{c^*})_{c^*} = Q_{c^*} \neq 0$ and thus Q^{c^*} is not only smooth and real-valued but also nonconstant. Thus $(Q^{c^*})^2$ is nonconstant, as well. So by the above, there exists a nonzero lattice vector $l \in \mathcal{L}\backslash\{0\}$ such that

$$\langle (Q^{c^*})^2, E_{Fl} \rangle \neq 0 \,.$$

Since it was assumed that $Q_{-Fl} = 0$ for all $l \in \mathcal{L}\backslash\{0\}$ the second partial wave invariant with respect to $-l$ is given by Theorem 5.8 as

$$\mathsf{wi}_{2,-l}(Q) = \sum_{c \in (-l)[0,0]}^{Q} 1 = \langle \sum_{c_1, c_2 \in l^\perp \backslash \{0\}} Q_{c_1} Q_{c_2} E_{c_1+c_2}, E_{Fl} \rangle = \langle (Q^{c^*})^2, E_{Fl} \rangle \neq 0 \,.$$

Because there is a nonvanishing partial wave invariant there must be nonisospectral translation-invariant connections by Corollary 4.39. □

6.5 Hearing Potentials

In the preceding sections we have studied to what extend the connections are spectrally determined by a potential. In this section we will ask the converse: Given some connection a is the potential Q determined by the spectrum of $\Delta_a^{\mathrm{D}} + Q$? We will mainly show that the results of [GGKW08] hold despite the sign error in [GGKW08], recall Remark 4.19. This is not unexpected, confer Remarks 4.33 and 4.49.

Definition 6.30. The *even part* of a smooth potential is defined as

$$Q^+ := \frac{1}{2}(Q + \check{Q}) \,,$$

where $\check{Q}(x) := Q(-x)$ as in Definition 1.25. The *odd part* of a smooth potential is defined as

$$Q^- := \frac{1}{2}(Q - \check{Q}) \,.$$

We have $Q = Q^+ + Q^-$.

Recall from Lemma 1.28 that a translation-invariant connection $a \in \mathbb{R}^{n'}$ is weakly $\mathbb{Z}_2$-invariant if $a(\mathcal{L}) \subset \mathbb{Z}/2$. For such a special connection parts of the potential can be recovered from the spectrum.

Theorem 6.31 ([GGKW08, Theorem 1.2]).
If $\mathcal{L}$ is nondegenerate, the Chern invariant factors of the line bundle ω all 1 and the translation-invariant connection a is weakly $\mathbb{Z}_2$-invariant, then the even part Q^+ of every potential Q is determined by $\mathrm{Spec}_a(Q,\omega)$. If Q is even, then Q is determined by $\mathrm{Spec}_a(Q,\omega)$.

Proof. Let $d \in |\mathcal{L}|\backslash\{0\}$ be arbitrary. Since $\mathcal{L}$ is nondegenerate there are only two lattice vectors $\pm l$ of length d. Since the connection a is weakly $\mathbb{Z}_2$-invariant we have $E_a(l) = E_{-a}(l) = \pm 1$ and it follows that the first small wave invariant is

$$\mathsf{wi}_{1,d}(a,Q) = E_a(l)\sigma_l \cdot \Big(Q_{-Fl} + Q_{Fl}\Big).$$

Let P denote another potential with the same spectrum as Q. Since all Chern invariant factors are 1 the map $F\colon \mathcal{L} \to \mathcal{L}'$ is surjective and we conclude from

$$\mathsf{wi}_{1,d}(a,Q) = \mathsf{wi}_{1,d}(a,P) \qquad \text{that}$$
$$(Q^+)_c = \frac{1}{2}(Q_c + Q_{-c}) = \frac{1}{2}(P_c + P_{-c}) = (P^+)_c \qquad \text{for all } c \in \mathcal{L}'.$$

Hence, all Fourier coefficients of the even part of P coincide with those of Q, thus $P^+ = Q^+$.

Further, the even and odd parts of Q are L^2-orthogonal and thus

$$\|Q\|_{\mathrm{L}^2} = \|Q^+\|_{\mathrm{L}^2} + \|Q^-\|_{\mathrm{L}^2}.$$

The L^2-norm of the potential is spectrally determined by the heat invariants and if we have an even potential $Q^+ = Q$ and a potential P isospectral to Q it follows that

$$\|Q^+\|_{\mathrm{L}^2} = \|Q\|_{\mathrm{L}^2} = \|P\|_{\mathrm{L}^2} = \|P^+\|_{\mathrm{L}^2} + \|P^-\|_{\mathrm{L}^2}.$$

Because $P^+ = Q^+$ we have $P^- = 0$. □

Theorem 6.32 ([GGKW08, Theorem 1.3]).
If the Chern invariant factors of ω are all 1, then every potential is uniquely determined by its ω-Bloch spectrum, recall Definition 1.36.

Proof. Let $d \in |\mathcal{L}|\backslash\{0\}$ and denote by $l_1, \dots, l_h \in \mathcal{L}$ all lattice vectors of length d in $\mathcal{L}$. For any h-tuple $a = (a_1, \dots, a_h) \in (\mathbb{R}^{n'})^h$ of translation-invariant connections, the vector $W = (\mathsf{wi}_{1,d}(a_1,Q), \dots, \mathsf{wi}_{1,d}(a_h,Q)$ of first small wave invariants is a spectral invariant of the ω-Bloch spectrum. Further, we have with $w = (\sigma_{l_1}\mathsf{wi}_{1,l_1}(Q), \dots, \sigma_{l_h}\mathsf{wi}_{1,l_h}(Q))$ that $W = V \cdot w$ with

$$V := \begin{pmatrix} E_{a_1}(l_1) & \cdots & E_{a_1}(l_h) \\ \vdots & \ddots & \vdots \\ E_{a_h}(l_1) & \cdots & E_{a_h}(l_h) \end{pmatrix}.$$

If we choose $a_1 = 0$, a_2 such that all $E_{a_2}(l_i)$ are pairwise distinct and $a_i = (i-1)\cdot a_2$ for $i > 2$ then V is a Vandermonde matrix with nonvanishing determinant. Thus, V is invertible and the small partial wave invariants $\mathsf{wi}_{1,l_i}(Q)$ are spectrally determined because the $\sigma_{l_i} = e_{l_i}(l_i/2)$ is part of the known data.

Since $\mathsf{wi}_{1,l_i}(Q) = Q_{-Fl_i}$ and since F is surjective we have that all Fourier coefficients of Q are spectrally determined by the ω-Bloch spectrum. □

The proof of this Theorem in [GGKW08, page 2474] is identical our proof given above. However, the signatures σ_{l_i} were forgotten in [GGKW08] (with no effect on the result).

With our notation of partial wave invariants the proof of the previous Theorem, as presented above, shows more:

Theorem 6.33. For every smooth potential on an even-dimensional torus with nondegenerate line bundle ω not just the (small) wave invariants but the (small) partial wave invariants individually are spectrally determined by the ω-Bloch spectrum.

Recall from Example 5.16 that $\mathrm{Spec}_a(Q,\omega) = \mathrm{Spec}_{-a}(\check{Q},\omega)$. Thus, for a weakly $\mathbb{Z}_2$-invariant connection a we have

$$\mathrm{Spec}(a,Q) = \mathrm{Spec}(a,\check{Q}) \qquad \text{for all potentials } Q,$$

because in this case $[a] = [-a]$. In particular, a single connection does not, in general, determine the potential Q.

The following theorem is slightly more general than [GGKW08, Theorem 4.9], because there it is assumed that $a = 0$.

Theorem 6.34. If M is a two-dimensional torus, $\mathcal{L}$ nondegenerate, the only Chern invariant factor $r_1 = 1$ and the translation-invariant connection a weakly $\mathbb{Z}_2$-invariant, then the squares of the odd parts of the one-dimensional potentials of Q are determined by $\mathrm{Spec}_a(Q,\omega)$, that is:

$$((Q^c)^-)^2 = ((P^c)^-)^2 \qquad \text{for all } c \in \mathcal{L}'\backslash\{0\},$$

provided Q and P are isospectral.

Proof. Since $\mathcal{L}$ is nondegenerate we can use the simple wave invariants of Theorem 5.13. Let $l \in \mathcal{L}\backslash\{0\}$. Since M is two-dimensional there is, up to scale, exactly one $d \in \mathcal{L}'$ with $d(l) = 0$ and we have

$$\mathsf{wi}^{\mathrm{s}}_{2,l}(Q) = \sum_{c\in l[0,0]}^{Q} 1 = \langle \sum_{c_1(l)=0=c_2(l)} Q_{c_1}Q_{c_2}E_{c_1+c_2}, E_{-Fl}\rangle = \langle (Q^d)^2, E_{-Fl}\rangle + 2Q_0Q_{-Fl}\,.$$

We abbreviate $q \coloneqq Q^d$ and with $E_a(\pm l) \in \pm 1$ by $a(\mathcal{L}) \subset \mathbb{Z}/2$ we have that

$$\mathsf{wi}_{2,|l|}(a,Q) = E_a(l)\sigma_l\Big(\langle q^2, E_{Fl} + E_{-Fl}\rangle - 2Q_0(Q_{Fl} + Q_{-Fl})\Big).$$

is determined by $\mathrm{Spec}_a(Q,\omega)$, because $\mathcal{L}$ is nondegenerate. We already know from Theorem 6.31 that the even part Q^+ of Q is spectrally determined, hence so are all $Q_{Fl} + Q_{-Fl}$. It follows that

$$\langle q^2, E_{Fl} + E_{-Fl}\rangle = \langle (q^+ + q^-)^2, E_{Fl} + E_{-Fl}\rangle = \langle (q^+)^2 + 2q^+q^- + (q^-)^2, E_{Fl} + E_{-Fl}\rangle$$

is a spectral invariant. We have $\langle 2q^+q^-, E_{Fl} + E_{-Fl}\rangle = 0$. Additionally, since Q^+ is spectrally determined and $q^+ = (Q^d)^+ = (Q^+)^d$ we have that $(q^+)^2$ is also spectrally determined. It follows that

$$\langle (q^-)^2, E_{Fl} + E_{-Fl}\rangle = 2\langle (q^-)^2, E_{Fl}\rangle$$

is determined by $\mathrm{Spec}_a(Q,\omega)$ as well. Since $r_1 = 1$ the map F is surjective and thus all Fourier coefficients of $(q^-)^2 = ((Q^d)^-)^2$ are spectrally determined. □

Appendix A

z-Derivatives

The goal of this section is to calculate the z-derivatives at $z = 0$ of the functions

$$v\colon \mathbb{R}^{n-1} \supset B^{n-1}_{\sqrt{2}}(0) \to \mathbb{R} \qquad \text{with} \qquad v(z) \coloneqq \kappa^{3-n}(z) = (1-|z|^2/4)^{\frac{n-3}{2}} \quad \text{and}$$
$$\omega\colon \mathbb{R}^{n-1} \supset B^{n-1}_{\sqrt{2}}(0) \to \mathbb{R}^n \qquad \text{with} \qquad \omega(z) \coloneqq R_l y(z)\,.$$

R_l is an orthogonal linear map with $R_l e_n = l/|l|$ and $y(z) \coloneqq (z/\kappa(z), 1-|z|^2/2)$ with $\kappa(z) \coloneqq (1-|z|^2/4)^{-1/2}$.

We have used some of those derivatives in the computation of the first two wave invariants in Example 4.29. The MATHEMATICA notebook needs a general algorithm to determine those derivatives to compute higher wave invariants.

Definition A.1 (z-multiindices).
In this section all multiindices $\alpha \in \mathbb{N}_0^{n-1}$ have length $n-1$, where $\mathbb{N}_0 \coloneqq \mathbb{N} \cup \{0\}$. We write

$$\partial_z^\alpha \coloneqq \partial_{z_1}^{\alpha_1} \circ \cdots \circ \partial_{z_{n-1}}^{\alpha_{n-1}}\,.$$

Given any multiindex $\alpha = (\alpha_1, \ldots, \alpha_h) \in \mathbb{N}^{n-1}$ the *factorial* is given by

$$\alpha! \coloneqq \alpha_1! \cdots \alpha_{n-1}!\,.$$

Remark A.2 (Double factorial).
The *double factorial* is defined recursively for some $k \in \mathbb{N}$ as

$$k!! \coloneqq k \cdot (k-2)!! \qquad \text{with } 0!! \coloneqq 1 \text{ and } 1!! \coloneqq 1.$$

Explicitly, this means $k!! \coloneqq \prod_{0 \le i < k/2}(k-2i)$. The double factorial $(k-1)!!$ of an even $k \in \mathbb{N}$ gives the number of possibilities to group k distinct elements of a set into pairs. Further, set for a negative $k \in \mathbb{Z}$ that

$$k!! \coloneqq \frac{(k+2)!!}{k+2}\,.$$

For an $(n-1)$-multiindex α define $\alpha!! \coloneqq \alpha_1!! \cdots \alpha_{n-1}!!$.

Lemma A.3 (Derivatives of v).
The derivative $\partial^\alpha v_{|z=0}$ is only nonvanishing for even multiindices: If there is some multiindex γ with $\alpha = 2\gamma$ then

$$\partial^\alpha v_{|z=0} = \frac{(\alpha-1)!!}{2^{|\alpha|}} \prod_{i=1}^{|\alpha|/2} (2i+1-n)\,.$$

If there is no such γ then

$$\partial^\alpha v_{|z=0} = 0\,.$$

Proof. Define $h(j)(z) \coloneqq (1-\frac{|z|^2}{4})^{\frac{n-3}{4}-j} \cdot \prod_{i=1}^{j} \frac{3-n+2(i-1)}{4}$ such that $\partial^\alpha v = \partial^\alpha h(0)$ and

$$\begin{aligned}\partial_k h(j) &= (\tfrac{n-3}{2} - j)\cdot(-z_k/2)(1-\tfrac{|z|^2}{4})^{\frac{n-3}{4}-j-1} \cdot \textstyle\prod_{i=1}^{j} \frac{3-n+2(i-1)}{4} \\ &= z_k(1-\tfrac{|z|^2}{4})^{\frac{n-3}{4}-(j+1)}(\tfrac{3-n}{4}+\tfrac{2j}{4}) \cdot \textstyle\prod_{i=1}^{j} \frac{3-n+2(i-1)}{4} = z_k \cdot h(j+1)\,.\end{aligned}$$

If we call i the z_k-*order* of $z_k{}^i\, h(j)$ then applying ∂_k to $z_k{}^i\, h(j)$ gives terms of z_k-order $i+1$ and $i-1$. This means that if there is an index k such that α_k is odd then the z_k-order of all terms in $\partial^\alpha v$ is odd. In particular, $\partial^\alpha v(0) = 0$.

If, however, $\alpha = 2\gamma$ then those terms remain where the z_k-factor generated by one derivative ∂_k is removed by another ∂_k. In other words, we have to group the α_k derivatives into pairs. There are $(\alpha_k - 1)!!$ such pairings for each index k and therefore

$$\partial^\alpha v(0) = (\alpha_1 - 1)!! \cdots (\alpha_{n-1} - 1)!! \cdot h(|\alpha|/2)(0)\,. \qquad \square$$

Remark A.4. Note that for $\alpha = 2\gamma$ we also have

$$\partial^\alpha v_{|z=0} = \frac{(\alpha-1)!!}{2^{|\alpha|/2}} \operatorname{Pochhammer}\Big(\frac{3-n}{2}, \frac{|\alpha|}{2}\Big) = \frac{(\alpha-1)!!}{2^{|\alpha|}} \frac{\Gamma(\frac{3-n+|\alpha|}{2})}{\Gamma(\frac{3-n}{2})}\,.$$

However, those expressions are not useful for evaluating the wave invariants because they do not (immediately) give explicit rational numbers.

Lemma A.5.
With $c_i^\alpha \coloneqq -2(\alpha - 1 + e_i)!! \cdot (|\alpha| - 4)!! \cdot 2^{-|\alpha|}$ we have for

$$y(z) \coloneqq \Big((1-|z|^2/4)^{-1/2} \cdot z, 1 - |z|^2/2\Big) \in \mathbb{R}^{n-1} \times \mathbb{R} \qquad \text{that}$$

$$\partial^\alpha y_{|z=0} = \begin{cases} e_n & \text{for } \alpha = 0 \\ -e_n & \text{for } \alpha = 2e_i \text{ with some } i \in \{1,\dots,n-1\} \\ c_i^\alpha e_i & \text{for } \alpha = 2\gamma + e_i \text{ with some multiindex } \gamma \text{ and} \\ 0 & \text{otherwise.} \end{cases}$$

Proof. Similarly to the proof of Lemma A.3 let $b(j)(z) \coloneqq (1-|z|^2/4)^{1/2-j} \cdot \prod_{i=1}^{j} \frac{2i-3}{4}$ such that

$$\begin{aligned}\partial_k b(j) &= \Big(1-\frac{|z|^2}{4}\Big)^{1/2-j-1}\Big(-\frac{z_k}{2}\Big)\cdot\Big(\frac{1}{2}-j\Big)\prod_{i=1}^{j}\frac{2i-3}{4}\\ &= z_k\cdot\Big(1-\frac{|z|^2}{4}\Big)^{1/2-(j+1)}\Big(j/2-\frac{1}{4}\Big)\prod_{i=1}^{j}\frac{2i-3}{4} = z_k\cdot b(j+1)\,.\end{aligned}$$

Now, however, we have for $j<n$ that

$$y_j = z_j\cdot b(0)\,.$$

Counting the z_k-orders of the terms appearing in $\partial^\alpha y_j$ we obtain that $\partial^\alpha y_j(0) = 0$ unless α_k is even for all $k\neq j$ and α_j is odd. α_j must be odd because the z_j-order of y_j is 1.

Now, let $\alpha = 2\gamma + e_j$ and denote by $\hat\alpha \coloneqq \alpha - \alpha_j e_j$. Then

$$\partial^\alpha y_j(0) = \partial^{\hat\alpha}\partial_j{}^{\alpha_j}(z_j b(0))_{|z=0} = \alpha_j\cdot(\alpha_j-2)!!\cdot\partial^{\hat\alpha} b\Big((\alpha_j-1)/2\Big)_{|z=0}\,,$$

because there are α_j choices of ∂_j-derivatives to remove the existing z_j-factor in y_j and then $((\alpha_j-1)-1)!! = (\alpha_j-2)!!$ pairings of the remaining derivatives. Only those (identical) terms contribute to the derivative $\partial^\alpha y_j(0)$. Note that if $\alpha_j = 1$ then $(\alpha_j-2)!! = (-1)!! = 1$, as desired.

The remaining derivatives $\partial^{\hat\alpha}$ need to be grouped in pairs as well, giving $(\hat\alpha-1)!!$ nonvanishing terms. Therefore,

$$\begin{aligned}\partial^\alpha y_j(0) &= \alpha_j\cdot(\alpha_j-2)!!\cdot(\hat\alpha-1)!!\cdot b(|\hat\alpha|/2+(\alpha_j-1)/2)_{|z=0}\\ &= \alpha_j!!\cdot(\hat\alpha-1)!!\cdot b((|\alpha|-1)/2)_{|z=0} = (\alpha-1+e_j)!!\cdot\prod_{i=1}^{(|\alpha|-1)/2}\frac{2i-3}{4}\\ &= (\alpha-1+e_j)!!\cdot 2^{1-|\alpha|}\cdot\prod_{i=1}^{(|\alpha|-1)/2}(2i-3)\\ &= (\alpha-1+e_j)!!\cdot 2^{1-|\alpha|}\cdot(-1)\cdot(|\alpha|-4)!! = c_j^\alpha\,,\end{aligned}$$

because $\prod_{i=1}^{(|\alpha|-1)/2}(2i-3) = -(|\alpha|-4)!!$.

Finally, note that trivially $\partial^\alpha y_n(0) = 1$ for $\alpha = 0$ and $\partial^\alpha y_n(0) = -1$ for $\alpha = 2e_i$. For all other α we have $\partial^\alpha y_n(0) = 0$. Altogether, the claim follows.□

With Lemma A.5 we obtain the z-derivatives of ω. Recall that $\{W_1,\dots,W_{n-1}, l/|l|\}$ is an orthonormal basis that is mapped to the standard basis by the orthogonal linear map R_l^{-1}.

Theorem A.6. The functions

$$v\colon \mathbb{R}^{n-1} \to \mathbb{R} \qquad \text{and} \qquad \omega\colon \mathbb{R}^{n-1} \to \mathbb{R}^n$$

have the derivatives

$$\partial^\alpha_{z=0} v = \begin{cases} 0 & \text{if there is an } i \in \{1,\dots,n-1\} \text{ such that } \alpha_i \text{ is odd and} \\ \frac{(\alpha-1)!!}{2^{|\alpha|}} \prod_{i=1}^{|\alpha|/2} (2i+1-n) & \text{otherwise and} \end{cases}$$

$$\partial^\alpha_{z=0} \omega = \begin{cases} l/|l| & \text{for } \alpha = 0 \\ -l/|l| & \text{for } \alpha = 2e_i \text{ with some } i \in \{1,\dots,n-1\} \\ c_i^\alpha W_i & \text{for } \alpha = 2\gamma + e_i \text{ with some multiindex } \gamma \text{ and} \\ 0 & \text{otherwise} \end{cases}$$

with $c_i^\alpha := -2(\alpha - 1 + e_i)!! \cdot (|\alpha| - 4)!! \cdot 2^{-|\alpha|}$. In particular,

$$\omega(0) \cdot l = |l| \qquad \text{and} \qquad \partial^2_{z_i} \omega \cdot l_{|z=0} = -|l| \qquad \text{for any } i \in \{1,\dots,n-1\} \text{ and}$$
$$\partial^\alpha \omega \cdot l_{|z=0} = 0 \qquad \text{for all other } \alpha.$$

Remark A.7. In the computation of the first two wave invariants we have abbreviated

$$K(z) := \langle \omega(z), l \rangle \cdot \omega(z)$$

and we needed some derivatives for this function at $z = 0$. It is trivial that

$$K(0) = l\,.$$

For the first derivative we have

$$\partial_{z_i=0} K(z) = \langle \partial_{z_i=0}\omega, l\rangle l/|l| + |l| \partial_{z_i=0}\omega = 0 + |l| W_i$$

because $c_i^{e_i} = 1$. Without Einstein summation we have

$$\partial^2_{z_i=0} K = \langle \partial^2_{z_i=0}\omega, l\rangle l/|l| + 2\langle \partial_{z_i=0}\omega, l\rangle \partial_{z_i=0}\omega + |l| \partial^2_{z_i=0}\omega$$
$$\langle -l/|l|, l\rangle l/|l| + |l|(-l/|l|) = -2l$$

and therefore

$$\Delta_{z=0} K = -2(n-1) l\,.$$

Furthermore, we need to write the z-Laplacian

$$\Delta := \sum_{i=1}^{n-1} \partial_{z_i}^2$$

in such a way that we can use Theorem A.6 to compute it. In the construction of the k-th wave invariants we need to apply the z-Laplacian up to k times, which gives sums of the form

$$\Delta^k := \sum_{i_1,\dots,i_k=1}^{n-1} \partial_{z_{i_1}}^2 \cdots \partial_{z_{i_k}}^2 .$$

To apply the derivatives in summary A.6 to sums of this form we need to convert these sums into sums where all indices are pair-wise distinct:

$$\Delta^k = \Big(\alpha_1 \sum_{i_1\neq\cdots\neq i_k=1}^{n-1} \partial_{z_{i_1}}^2 \cdots \partial_{z_{i_k}}^2 + \alpha_2 \sum_{i_1=i_2\neq\cdots\neq i_k=1}^{n-1} \partial_{z_{i_1}}^2 \cdots \partial_{z_{i_k}}^2 + \cdots + \alpha_h \sum_{i_1=\cdots=i_k=1}^{n-1} \partial_{z_{i_1}}^2 \cdots \partial_{z_{i_k}}^2 \Big).$$

Here, h is the number of *partitions* $p = \{p_1, \dots, p_s\}$ of k into nonnegative integers with $p_1 + \cdots + p_s = k$ and α_p is the multiplicity of the sum corresponding to the partition p.

Definition A.8 (Partition).
A *partition* of a natural number k is tuple $(p_1, \dots, p_s)$ of natural numbers with $p_1 \geq \cdots \geq p_s > 0$ such that $p_1 + \cdots + p_s = k$. The set of all partitions of k will be denoted by $P(k)$ and the *length* of a partition shall be denoted by $L(p) := s$. For a partition $p \in P(k)$ denote by $T(p)$ a tuple of the multiplicities of the integers appearing in p. For example,

$$T(3,2,1,1) = (1,1,2) \qquad \text{and} \qquad T(7) = (1)\,.$$

Theorem A.9. The k-th exponent of the z-Laplacian can be rewritten as

$$\Delta_z^k = \sum_{p\in P(k)} \sum_{i_1,\dots,i_{L(p)}=1}^{n-1\,\mathrm{d}} \mathrm{CM}(p) \cdot \partial_{z_{i_1}}^{2p_1} \cdots \partial_{z_{i_{L(p)}}}^{2p_{L(p)}} ,$$

where the indices in the sums

$$\sum_{i_1,\dots,i_h=1}^{n-1\,\mathrm{d}} \quad \text{are pairwise-distinct, } i_r \neq i_s \text{ for all } 1 \leq r,s \leq h \text{ and}$$

$$\mathrm{CM}(p) := \frac{k!}{p! \cdot T(p)!} \qquad \text{is a } \textit{custom multinomial}.$$

Proof. It is clear that the Laplacians Δ_z^k can be expressed as a sum over sums with unequal indices and that such a sum must run over the set of partitions of k. It remains to show that $CM(p)$ is indeed the multiplicity of such sums. The multiplicity is given by the number of possibilities to choose p_1 indices out of k indices, p_2 indices out of $k-p_1$ indices until we have grouped all indices according to the partition p. This gives the multinomial

$$\binom{k}{p_1}\cdot\binom{k-p_1}{p_2}\cdots\binom{k-p_1-\cdots-p_{L(p)-1}}{p_{L(p)}} = \frac{k!}{p_1!\cdots p_{L(p)}!}\,.$$

However, the multinomial would over-count the multiplicity of the sum corresponding to the partition p, because groups of indices of equal size can be interchanged. Therefore, the multiplicity of the sum corresponding to p is given by

$$\frac{k!}{p!\cdot T(p)!} = \mathrm{CM}(p)\,.$$

□

Example A.10.

$$\Delta_z = \sum_{i_1=1}^{n-1}\partial_{z_{i_1}}^2 = \sum_{i_1=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^2$$

$$\Delta_z^2 = \sum_{i_1,i_2=1}^{n-1}\partial_{z_{i_1}}^2\partial_{z_{i_2}}^2 = \sum_{i_1=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^4 + \sum_{i_1,i_2=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^2\partial_{z_{i_2}}^2$$

$$\Delta_z^3 = \sum_{i_1,i_2,i_3=1}^{n-1}\partial_{z_{i_1}}^2\partial_{z_{i_2}}^2\partial_{z_{i_3}}^2 = \sum_{i_1=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^6 + 3\sum_{i_1,i_2=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^4\partial_{z_{i_2}}^2 + \sum_{i_1,i_2,i_3=1}^{n-1\,\mathrm{d}}\partial_{z_{i_1}}^2\partial_{z_{i_2}}^2\partial_{z_{i_3}}^2$$

Appendix B

τ-Integration

In this chapter we will study two algorithms, Algorithm I and Algorithm P needed to compute the τ-integrals appearing in the computation of the wave invariants. The Mathematica implementation of those algorithms is given in Appendix D and this chapter is intended to be a guide to this implementation.

We will start this chapter with some notation and the computation of an exemplary τ-integral that appears in the computation of the second wave invariant. Following the example we will construct an algorithm suitable to integrate all τ-integrals needed for the wave invariants. After that some simplifications of resulting integrals are discussed.

B.1 Multiindices

Definition B.1 (Multiindex).
We call the elements $e \in \mathbb{Z}^\lambda$ *multiindices* of *length* $\lambda \in \mathbb{N}$ and denote by $\mathrm{BM}^\lambda := \{0,1\}^\lambda$ the set of *binary multiindices*. We call a multiindex *e increasing* if

$$e_1 \leq \cdots \leq e_\lambda \,.$$

For $k \in \mathbb{Z}$ let $e + k := (e_1 + k, \ldots, e_\lambda + k)$ and write $e \geq k$ if $e_i \geq k$ for all $i = 1, \ldots, \lambda$. Similarly, we say that two multiindices $e, f \in \mathbb{Z}^\lambda$ satisfy $e \leq f$ if $e_i \leq f_i$ for all $i = 1, \ldots, \lambda$. Further, set $\tau^e := \tau_1^{e_1} \cdots \tau_\lambda^{e_\lambda}$.

If $\lambda > 1$ we can *drop* the first index in a multiindex $e \in \mathbb{Z}^\lambda$, denote this by

$$\dagger e := (e_2, \ldots, e_\lambda) \in \mathbb{Z}^{\lambda-1} \,.$$

For an integer $1 \leq H < \lambda$ we set $\dagger^H e := \dagger \cdots \dagger e = (e_{H+1}, \ldots, e_\lambda)$ and if $H = \lambda$ we set $\tau^{\dagger^\lambda e} := 1$. (We use the dagger symbol because we cut-off the first index of a given multiindex.)

A tuple $(b_1, \dots, b_q) \in (\mathrm{BM}^\lambda)^q$ of binary multiindices is said to be in *flag-form* if each binary multiindex b_i is increasing and if

$$b_i \geq b_{i+1} \qquad \text{for all } i = 1, \dots, q-1.$$

For such a tuple b we define that dropping the first index applies to each element of b:

$$\dagger b \coloneqq (\dagger b_1, \dots, \dagger b_q)\,.$$

Recall that Q_c denotes the Fourier coefficient of the potential Q for $c \in \mathcal{L}'$ and $E_c \coloneqq \mathrm{e}^{-\tilde{c}}$ the elements of the corresponding orthonormal basis, confer Definition 2.2.

Definition B.2. For a smooth potential Q and $c \in \mathcal{L}'^q$ we write

$$Q_c \coloneqq Q_{c_1} \cdots Q_{c_q} \qquad \text{and} \qquad E_c(x) \coloneqq E_{c_1}(x) \cdots E_{c_q}(x) = E_{c_1+\dots+c_q}(x)\,.$$

If $1 \leq h \leq q$ and $b \in (\mathrm{BM}^\lambda)^q$ is a tuple of binary multiindices then we set

$$E_c^h(l\tau^b) \coloneqq E_{c_h}(l\tau^{b_h}) \cdots E_{c_q}(l\tau^{b_q}) \qquad \text{and} \qquad E_c^{q+1}(l\tau^b) \coloneqq 1\,.$$

Further, if $c_i \in \mathcal{L}'$ and $d = \{X_1, \dots, X_h\} \subset \mathbb{R}^n$ is a (possibly empty) set of vectors then let $c_i(d) \coloneqq c_i(X_1) \cdots c_i(X_h)$. If $c \in \mathcal{L}'^q$ is a tuple of dual lattice vectors and $d = (d_1, \dots, d_q)$ some tuple of sets of vectors then abbreviate

$$c(d) \coloneqq c_1(d_1) \cdots c_q(d_q)\,.$$

The notation

$$Q(x + l\tau^{b_i}, d) \qquad \text{with } d = \{X_1, \dots, X_j\}$$

denotes the j-th derivative of Q in the direction of the vectors in d:

$$Q(x + l\tau^{b_i}, d) = \frac{\partial}{\partial x^\alpha} Q(x + l\tau^{b_i}) \cdot X_\alpha \coloneqq \frac{\partial}{\partial x^{\alpha_1}} \cdots \frac{\partial}{\partial x^{\alpha_j}} Q(x + l\tau^{b_i}) X_{1,\alpha_1} \cdots X_{j,\alpha_j}$$

with the Einstein convention for the multiindex α. If d is the empty set, then we simply have no derivative,

$$Q(x + l\tau^{b_i}, \emptyset) = Q(x + l\tau^{b_i})\,.$$

Before we can proceed to compute τ-integrals we first study in what form the τ-variables appear in each summand of the wave invariant. We show that the arguments of the potentials Q must be in *flag-form* for every summand of the wave invariants.

Lemma B.3. If we write A_i of $a_i = a_0 \frac{\mathrm{i}}{2} t A_i$ in expanded form then every summand of A_i is of the form

$$C \cdot Q(x + t\omega - \tau^{b_1} t\omega, d_1) \cdots Q(x + t\omega - \tau^{b_h} t\omega, d_q)\,,$$

where C is free of Q, the $d_i \subset \{e_i, \omega\}$ are finite sets denoting the derivatives of Q, $b \in (\mathrm{BM}^\lambda)^q$ is in flag-form and $q \leq i$.

Of course, b is only in flag-form if the order of the b_i is chosen appropriately. As a side effect we see that the derivatives of the potentials Q do not depend on x or t.

Proof. The definition of a_i can be found in Section 4.4. a_0 contains no potential and the potential is multiplied to a_{i-1} exactly once via the application of the Schrödinger operator $\Delta_a^{\mathrm{D}} + Q$ within the wave operator $\Box$. In particular,

$$a_1 = C_1 \cdot Q(x + (1 - \tau_1) t\omega) + C_2\,,$$

where C_1 and C_2 are expressions free of the potential Q. Expanding the argument of the potential Q gives

$$a_1 = C_1 \cdot Q(x + t\omega - \tau_1 t\omega) + C_2\,.$$

In other words, the first summand is of the desired form with $d_1 = \emptyset$ and $b = ((1))$ trivially in flag-form.

Inductively we are now assuming that a_i consists of summands of the form

$$C \cdot Q(x + t\omega - \tau^{b_1} t\omega, d_1) \cdots Q(x + t\omega - \tau^{b_h} t\omega, d_h)\,,$$

where $0 \leq h \leq i$ and $(b_1, \ldots, b_h)$ is in flag-form. If we apply the wave operator to a_i to compute a_{i+1} two types of summands are generated: On the one hand derivatives are applied, which change C and the d_i but leave the first, nonderivative arguments of the potential unchanged and which do not add another potential to the summands. This gives summands of the form

$$\begin{aligned}
&C' \cdot Q(x + t\omega - \tau^{b_1} t\omega, d_1') \cdots Q(x + t\omega - \tau^{b_h} t\omega, d_h') \\
&\to_{i+1} C' \cdot Q(x + (1 - \tau_{i+1}) t\omega + \tau_{i+1} t\omega - \tau^{b_1} \tau_{i+1} t\omega, d_1') \\
&\qquad \cdots Q(x + (1 - \tau_{i+1}) t\omega + \tau_{i+1} t\omega - \tau^{b_h} \tau_{i+1} t\omega, d_h') \\
&\qquad = C' \cdot Q(x + t\omega - \tau^{b_1'} t\omega, d_1') \cdots Q(x + t\omega - \tau^{b_h'} t\omega, d_h')\,,
\end{aligned}$$

where we use the Notation 4.27. Here, b' is obtained from b by adding a 1 to every b_i. Of course, b' is again in flag-form.

On the other hand, summands of a_{i+1} are obtained by multiplication with the potential.

$$\begin{aligned}
&C \cdot Q(x)Q(x + t\omega - \tau^{b_1} t\omega, d_1) \cdots Q(x + t\omega - \tau^{b_h} t\omega, d_h) \\
&\quad \to_{i+1} C' \cdot Q(x + (1 - \tau_{i+1})t\omega) \cdot \\
&\qquad\qquad Q(x + (1 - \tau_{i+1})t\omega + \tau_{i+1} t\omega - \tau^{b_1} \tau_{i+1} t\omega, d_1) \cdots \\
&\qquad\qquad\quad Q(x + (1 - \tau_{i+1})t\omega + \tau_{i+1} t\omega - \tau^{b_h} \tau_{i+1} t\omega, d_h) \\
&\qquad = C' \cdot Q(x + t\omega - \tau_{i+1} t\omega) \cdot \\
&\qquad\qquad Q(x + t\omega - \tau^{b_1} \tau_{i+1} t\omega, d_1) \cdots Q(x + t\omega - \tau^{b_h} \tau_{i+1} t\omega, d_h) \,.
\end{aligned}$$

This summand equals

$$C' \cdot Q(x + t\omega - \tau^{b'_1} t\omega, d_1) \cdots Q(x + t\omega - \tau^{b'_{h+1}} t\omega, d_{h+1}) \,.$$

But here we not only add a 1 to every b_k. We also add the vector $b'_{h+1} := e_{i+1}$ to b (and set $d_{h+1} := \emptyset$). This b' is again in flag-form.

This proves that every summand of a_i is indeed of the form above and that the τ-exponents within Q are in flag-form.

The fact that the derivatives d_i must be a subset of $\{e_i, \omega\}$ follows from the form of the arguments of Q. Two types of derivatives are applied to Q: ∂_{x_k} and ∂_t. In these two cases we have that

$$\begin{aligned}
&\partial_{x_k} Q(x + t\omega - \tau^{b_k} t\omega, d_k) = Q(x + t\omega - \tau^{b_k} t\omega, d_k \cup \{e_k\}) \qquad \text{and} \\
&\partial_t Q(x + t\omega - \tau^{b_k} t\omega, d_k) = Q(x + t\omega - \tau^{b_k} t\omega, d_k \cup \{\omega\})(1 - \tau^{b_k}) \,.
\end{aligned}$$

Either way, the derivatives are of the claimed form. □

Recall that the wave invariants are sums of $H(i, j, k)$, see Section 4.4.

Lemma B.4 (Flag-form).
If we write $H(i, j, k)$ in expanded form then every summand of $H(i, j, k)$ is of the form

$$C \cdot Q(x + \tau^{b_1} l, d_1) \cdots Q(x + \tau^{b_q} l, d_q) \,,$$

where $b \in (\mathrm{BM}^\lambda)^q$ is in flag-form, $q \le k$, the derivatives satisfy $d_i \subset \{l, W_i, e_i\}$ and C is free of Q.

Proof. When computing the terms $H(i, j, k)$ we first substitute the arguments of a_i and then apply differential operators to the resulting expression. By Section 4.4 we first need

$$\begin{aligned}
&a_i(t, x + l, -\omega(z)) \qquad \text{which gives summands of the form} \\
&C' \cdot Q(x + l - t\omega + \tau^{b_1} t\omega, d_1) \cdots Q(x + l - t\omega + \tau^{b_h} t\omega, d_h) \,.
\end{aligned}$$

To such summands we apply ∂_t-derivatives, which may change the coefficient C' and the derivatives d_i (by adding $\omega(z)$) but do not alter the first argument of the potential. After the differentiation we replace t by $\langle\omega(z), l\rangle$. We obtain summands of the form

$$C'' \cdot Q(x + l - \langle\omega, l\rangle\omega + \tau^{b_1}\langle\omega, l\rangle\omega, d_1') \cdots Q(x + l - \langle\omega, l\rangle\omega + \tau^{b_h}\langle\omega, l\rangle\omega, d_h')\,,$$

where ω depends on z.

After that, z-Laplacians are applied. Again, those Laplacians can change the coefficient and the derivatives d_i' but leave the first argument of the potentials unchanged. Note that d_i' is a (possibly empty) set consisting, at this point, of e_i, $\omega(z)$ and derivatives of $\omega(z)$. The Laplacians are evaluated at $z = 0$ and by Theorem A.6

$$\langle\omega(0), l\rangle\omega(0) = \langle l/|l|, l\rangle l/|l| = l\,.$$

The derivatives of ω at $z = 0$ evaluate to 0, l or W_i (times some factor), also by Theorem A.6. Therefore, all summands in the wave invariants have the form

$$\begin{aligned} C''' \cdot Q(x + l - l + \tau^{b_1} l, d_1'') \cdots Q(x + l - l + \tau^{b_h} l, d_h'') \\ = C''' \cdot Q(x + \tau^{b_1} l, d_1'') \cdots Q(x + \tau^{b_h} l, d_h'')\,, \end{aligned}$$

where b is still in flag-form and $d_i'' \subset \{l, W_i, e_i\}$. □

B.2 First Integrals

So far we have shown that the τ-integrals appearing in the wave invariants are all of the form

$$\int_{[0,1]^\lambda} \tau^e \prod_{i=1}^{q} Q(x + l \cdot \tau^{b_i}, d_i)\,\mathrm{d}\tau\,,$$

where e is a multiindex of length λ, $b \in (\mathrm{BM}^\lambda)^q$ is a tuple of binary multiindices and the d_i are finite (and possibly empty) sets of vectors. By Lemma B.4 we can assume that the binary multiindices b are in *flag form*.

For such an expression S we call e the *τ-exponent* of S.

Those τ-variables that appear only in e but not within any of the arguments of the potential Q integrate very simply,

$$\tau_i^{e_i} \to \frac{1}{e_i + 1}\,.$$

We call such τ-variables *trivial* and we assume from now on that any τ-variable in the τ-integral appears in at least one Q. We will start by integrating some example integrals. The order of factors in the integrands may seem

unconventional. We will write the integrands in the order used in the MATHEMATICA notebook.

Example B.5. Summands that appear in the third partial wave invariant are, for example,

$$Q(x+l\tau_2)Q(x+l\tau_1\tau_2)\cdot\tau_2\cdot\frac{43}{32}\mathrm{i}|l|\,,\qquad \text{with}$$
$$e=(0,1)\,,\qquad b=\Big((0,1),(1,1)\Big)\qquad\text{and}\qquad d_1=d_2=\emptyset\,,$$

and

$$Q(x+l\tau_2,\{W_{i_1}\})Q(x+l\tau_1\tau_2,\{W_{i_1}\})\cdot\tau_1\tau_2^3\cdot\frac{-\mathrm{i}}{4}|l|^3\,,\qquad \text{with}$$
$$e=(1,3)\,,\qquad b=\Big((0,1),(1,1)\Big)\qquad\text{and}\qquad d_1=d_2=\{W_{i_1}\}\,.$$

Note that in the so-called *canonical order* used in MATHEMATICA the binary multiindices b are not in flag-form, the order of the elements of b (and d) has to be reversed. Since the τ-integral is invariant under permutations of b and d, we may assume that b is of the form

$$b=((1,1),(0,1))\qquad\text{corresponding to}\qquad Q(x+l\tau_1\tau_2,d_2)Q(x+l\tau_2,d_1)\tau^e\,.$$

To calculate the τ-integrals we write the potentials Q as Fourier series,

$$Q(x)=\sum_{c\in\mathcal{L}'}Q_cE_c(x)\,,$$

and then integrate each summand separately. This can be done by the following Lemmata.

Lemma B.6. We can interchange integration with respect to τ and the summation as a Fourier series,

$$\int_{[0,1]^\lambda}\tau^e\prod_{i=1}^q Q(x+l\tau^{b_i},d_i)\,\mathrm{d}\tau=\sum_{c\in\mathcal{L}'^q}Q_cE_c(x)\int_{[0,1]^\lambda}E_c(l\tau^b)\cdot\tau^e\cdot(-\tilde{c})(d)\,\mathrm{d}\tau\,.$$

Proof. This Lemma follows from Fubini's Theorem: Abbreviate $\Pi(x,\tau):=\prod_{i=1}^q Q(x+l\tau^{b_i},d_i)$, which is still smooth and periodic. $\Pi(x,\tau)$ has the Fourier series

$$\Pi(x,\tau)=\sum_{\alpha\in\mathcal{L}'}\sum_{\substack{c\in\mathcal{L}'^q\\ \sum c_i=\alpha}}Q_cE_c(x)\cdot E_c(l\tau^b)\cdot(-\tilde{c})(d)\,.$$

Thus,

$$\begin{aligned}\langle \int_{[0,1]^\lambda} \tau^e \Pi(\,.\,,\tau)\,\mathrm{d}\tau, E_\alpha\rangle &= \int_M \int_{[0,1]^\lambda} \tau^e \cdot \Pi(x,\tau)\overline{E_\alpha(x)}\,\mathrm{d}\tau\mathrm{d}x \\ = \int_{[0,1]^\lambda}\int_M \tau^e \cdot \Pi(x,\tau)\overline{E_\alpha(x)}\,\mathrm{d}x\mathrm{d}\tau &= \int_{[0,1]^\lambda} \tau^e \sum_{\substack{c\in\mathcal{L}'^q \\ \sum c_i=\alpha}} Q_c \cdot E_c(l\tau^b)\cdot(-\tilde{c})(d)\,\mathrm{d}x\mathrm{d}\tau \\ &= \sum_{\substack{c\in\mathcal{L}'^q \\ \sum c_i=\alpha}} Q_c \int_{[0,1]^\lambda} E_c(l\tau^b)\cdot\tau^e\cdot(-\tilde{c})(d)\,\mathrm{d}x\mathrm{d}\tau\end{aligned}$$

and the claim follows. □

We continue to use the Einstein convention "$\overset{\tau}{=}$" for τ-integrals of Notation 4.26 and omit the integral signs from our notation:

$$f(\tau) \overset{\tau}{=} g(\tau) \qquad \text{if} \qquad \int_{(0,1)^\lambda} f(\tau)\,\mathrm{d}\tau = \int_{(0,1)^\lambda} g(\tau)\,\mathrm{d}\tau\,,$$

where λ is the maximal index of any τ-variable appearing in either $f(\tau)$ or $g(\tau)$. Note that we are integrating over $(0,1)$ and thus superfluous integrations over nonappearing variables do not lead to errors. Lemma B.6 states that this notation is compatible with Fourier expansion.

The following lemma is technical but central for the τ-integration of this section. It integrates a single τ-variable. Its case distinction necessitates the complicated definition of the *cases* later on.

Lemma B.7. Let $c \in \mathcal{L}'$ denote some dual lattice vector, $0 \le e \in \mathbb{Z}^\lambda$ a nonnegative multiindex and $b_1 \in \mathrm{BM}^\lambda$ some binary multiindex with $b_{1,1} = 1$. Then

$$E_c(l\tau^{b_1})\tau^e \overset{\tau}{=} \begin{cases} \tau^{\dagger e}\cdot\frac{1}{e_1+1} & \text{for } c(l)=0 \\ \tau^{\dagger(e-(e_1+1)b_1)}\cdot e_1!\cdot\tilde{c}(l)^{-e_1-1} & \\ \quad -E_c(l\tau^{\dagger b_1})\sum_{i=0}^{e_1}\tau^{\dagger(e+(i-e_1-1)b_1)}\cdot\frac{e_1!}{i!}\tilde{c}(l)^{i-e_1-1} & \text{for } c(l)\neq 0. \end{cases}$$

If $c(l) \neq 0$ and $b_1 = (1)$ is of length $\lambda = 1$ then $E_c(l\tau^{\dagger b_1}) = 1$ and

$$E_c(l\tau^{b_1})\tau^e \overset{\tau}{=} -\sum_{i=1}^{e_1}\frac{e_1!}{i!}\tilde{c}(l)^{i-e_1-1}\,.$$

Proof. The integral is trivial if $c(l) = 0$, because then $E_c(l\tau^{b_1}) = 1$. To compute the case that $c(l) \neq 0$ we first compute the integral

$$\int_0^1 \mathrm{e}^{-\alpha u}u^k\,\mathrm{d}u \qquad \text{with } \alpha \neq 0 \text{ and } k \in \mathbb{N}_0.$$

To this end, find constants p_i with

$$\partial_u\Big(\mathrm{e}^{-\alpha u}\sum_{i=0}^{k} p_i u^i\Big) = -\alpha\mathrm{e}^{-\alpha u}\sum_{i=0}^{k} p_i u^i + \mathrm{e}^{-\alpha u}\sum_{i=1}^{k} i p_i u^{i-1}$$
$$= \mathrm{e}^{-\alpha u}(-\alpha p_k)u^k + \mathrm{e}^{-\alpha u}\sum_{i=0}^{k-1}\Big((i+1)p_{i+1} - \alpha p_i\Big)u^i \overset{!}{=} \mathrm{e}^{-\alpha u}u^k\,.$$

Thus, the leading coefficient must satisfy $p_k = -1/\alpha$. The other coefficients must cancel, $(i+1)p_{i+1} - \alpha p_i = 0$, which implies that $p_i = (i+1)p_{i+1}/\alpha$ and thus $p_{i-1} = ip_i/\alpha$. Inductively, it follows that $p_i = -\frac{k!}{i!}\alpha^{i-k-1}$. Hence,

$$\int_0^1 \mathrm{e}^{-\alpha u}u^k\,\mathrm{d}u = \sum_{i=0}^{k} p_i\mathrm{e}^{-\alpha} - p_0 = \sum_{i=0}^{k}\Big(-\frac{k!}{i!}\alpha^{i-k-1}\mathrm{e}^{-\alpha}\Big) + k!\alpha^{-k-1}\,.$$

If we rewrite the integrand of the τ-integral as $E_c(l\tau^{b_1})\tau^e = \mathrm{e}^{-\tilde{c}(l)\tau_1\tau^{\dagger b_{1,1}}}\cdot\tau_1^{e_1}\tau^{\dagger e}$ we can apply the u-integral above to the variable τ_1, the exponent $e_1 \geq 0$ and $\alpha = \tilde{c}(l)\tau^{\dagger b_1} \neq 0$:

$$E_c(l\tau^{b_1})\tau^e \overset{\tau}{=} \sum_{i=0}^{e_1}\Big(-\frac{e_1!}{i!}(\tilde{c}(l)\tau^{\dagger b_1})^{i-e_1-1}\mathrm{e}^{-\tilde{c}(l)\tau^{\dagger b_1}}\Big)\cdot\tau^{\dagger e} + e_1!(\tilde{c}(l)\tau^{\dagger b_1})^{-e_1-1}\cdot\tau^{\dagger e}$$
$$= \tau^{\dagger(e-(e_1+1)b_1)}\cdot e_1!\tilde{c}(l)^{-e_1-1} - E_c(l\tau^{\dagger b_1})\sum_{i=0}^{e_1}\tau^{\dagger(e+(i-e_1-1)b_1)}\cdot\frac{e_1!}{i!}\tilde{c}(l)^{i-e_1-1}$$

If $b_1 = (1)$ then $\tau^{\dagger b_1} = 1$ and $\tilde{c}(l\tau^{\dagger b_1}) \in 2\pi\mathrm{i}\mathbb{Z}$. Thus, $E_c(l\tau^{\dagger b_1}) = 1$ and

$$E_c(l\tau^{b_1})\tau^e \overset{\tau}{=} e_1!\tilde{c}(l)^{-e_1-1} - \sum_{i=0}^{e_1}\frac{e_1!}{i!}\tilde{c}(l)^{i-e_1-1} = -\sum_{i=1}^{e_1}\frac{e_1!}{i!}\tilde{c}(l)^{i-e_1-1}\,.$$

□

If there is more than one τ-variable we can apply Lemma B.7 repeatedly, where needed, to compute all τ-integrals. However, there are two problems with this approach, which shall be illustrated in the following examples. The first problem arises in the form of negative τ-exponents that appear if the exponent e is not strictly increasing, $e_i < e_{i+1}$.

Example B.8. Consider the τ-integral of

$$Q(x + \tau_1\tau_2 l, \{l\}) = \sum_{c\in\mathcal{L}'} Q_c E_c(x)\cdot E_c(\tau_1\tau_2 l)\cdot(-\tilde{c}(l))\,.$$

The derivative of Q with respect to l adds the factor of $-\tilde{c}(l)$ to the Fourier coefficients and, hence, for $c(l) = 0$ the Fourier summands vanish without τ-integration.

Let us apply Lemma B.7 to those summands with $c(l) \neq 0$:

$$E_c(\tau_1\tau_2 l) \overset{\tau}{=} \tau_1^{-1}\frac{1}{\tilde{c}(l)} - E_c(\tau_1 l)\cdot\tau_1^{-1}\cdot\frac{1}{\tilde{c}(l)}\,.$$

Now, because the τ-exponent $(0,0)$ was not strictly increasing, we have terms whose first τ-exponent is negative and we cannot apply Lemma B.7 to either of those two summands. In fact, either summand individually gives a divergent integral, confer Definition B.16. Overall the τ-integrals are well-defined, of course, because Q is smooth and integrated over a compact domain.

This may seem like a dead end for the τ-integration. However, it will turn out, at least for the first five wave invariants, that we can just leave the (superficially) divergent τ-integrals standing. They will cancel each other out.

The second problem that arises is that, in general, the k-th wave invariant has summands containing Q in up to k-th order. Although Lemma B.7 is simple enough the fact that we have to distinguish whether $c(l)$ vanishes or not leads to rather complicated combinatorics.

The following example is (up to the coefficient $-|l|^4/4$) the only term with higher than linear Q-order in the second wave invariant. The example is needed for the manual calculation of the second wave invariants in Section 4.7.1.

Example B.9. $$\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l) \overset{\tau}{=} \sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1(l)=0=c_2(l)}} Q_c E_c(x)\cdot\frac{1}{2}$$

Proof. First, write both instances of Q as a Fourier series,

$$\begin{aligned}\tau_2 Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l) &= \tau_2\sum_{c_1,c_2\in\mathcal{L}'} Q_{c_1}E_{c_1}(x)E_{c_1}(\tau_2 l)Q_{c_2}E_{c_2}(x)E_{c_2}(\tau_1\tau_2 l)\\ &= \sum_{c\in\mathcal{L}'^2} Q_c E_c(x)\cdot E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\cdot\tau_2\end{aligned}$$

Thus, the τ-integrand of interest is

$$E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\cdot\tau_2\,,$$

which has the multiindices $e=(0,1)$ and $b=((1,1),(0,1))$. b is in flag-form if we arrange the potentials inversely to the *canonical order* used by MATHEMATICA for the integrand. We apply Lemma B.7 and distinguish two cases: $c_1(l)=0$ and $c_1(l)\neq 0$. If $c_1(l)=0$, then

$$E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 = E_{c_2}(\tau_2 l)\tau_2$$

and we can use Lemma B.7 on the remaining integral. There are again two cases to distinguish: $c_2(l) = 0$ and $c_2(l) \neq 0$.

$$\begin{aligned}
&\text{If } c_2(l) = 0 \qquad E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 = \tau_2 \overset{\tau}{=} \frac{1}{2} \qquad \text{and} \\
&\text{if } c_2(l) \neq 0 \qquad E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 = E_{c_2}(\tau_2 l)\tau_2 \overset{\tau}{=} -\tilde{c}_2(l)^{-1}\,.
\end{aligned}$$

If, on the other hand, $c_1(l) \neq 0$ then Lemma B.7 yields

$$\begin{aligned}
E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 &\overset{\tau}{=} \left(\tilde{c}_1(l)^{-1} - E_{c_1}(l\tau_2)\tilde{c}_1(l)^{-1}\right)\cdot E_{c_2}(l\tau_2) \\
&= \frac{1}{\tilde{c}_1(l)}E_{c_2}(\tau_2 l) - \frac{1}{\tilde{c}_1(l)}E_{c_1+c_2}(\tau_2 l)\,.
\end{aligned}$$

Now, contrary to what one might expect, we have not two but *three* cases to consider: $c_2(l)$ might vanish, $c_2(l) = -c_1(l) \neq 0$ or $c_2(l)$ might satisfy neither of these two equations.

If $c_2(l) = 0$ then

$$E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 \overset{\tau}{=} \frac{1}{\tilde{c}_1(l)} - E_{c_1}(\tau_2 l)\frac{1}{\tilde{c}_1(l)} \overset{\tau}{=} \frac{1}{\tilde{c}_1(l)}\,,$$

if $c_2(l) = -c_1(l) \neq 0$ then

$$E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 \overset{\tau}{=} E_{-c_1}(\tau_2 l)\frac{1}{\tilde{c}_1(l)} - \frac{1}{\tilde{c}_1(l)} \overset{\tau}{=} -\frac{1}{\tilde{c}_1(l)}$$

and if $c_2(l)$ satisfies neither of those two cases then both $c_2(l) \neq 0$ and $(c_1 + c_2)(l) \neq 0$ and thus

$$E_{c_1}(\tau_1\tau_2 l)E_{c_2}(\tau_2 l)\tau_2 = 0\,.$$

So far, we have the following result

$$\begin{aligned}
&Q(x+\tau_1\tau_2 l)Q(x+\tau_2 l)\tau_2 \\
&\qquad \overset{\tau}{=} \sum_{\substack{c\in\mathcal{L}'^2 \\ c_1(l)=0=c_2(l)}} Q_c E_c(x)\cdot\frac{1}{2} \quad + \sum_{\substack{c\in\mathcal{L}'^2 \\ c_1(l)\neq 0=c_2(l)}} Q_c E_c(x)\cdot\frac{1}{\tilde{c}_1(l)} \\
&\qquad + \sum_{\substack{c\in\mathcal{L}'^2 \\ c_1(l)=0\neq c_2(l)}} Q_c E_c(x)\cdot\frac{-1}{\tilde{c}_2(l)} \quad + \sum_{\substack{c\in\mathcal{L}'^2 \\ c_1(l)=-c_2(l)\neq 0}} Q_c E_c(x)\cdot\frac{-1}{\tilde{c}_1(l)}
\end{aligned}$$

A variable substitution $c_1 \leftrightarrow c_2$ gives

$$\sum_{\substack{c\in\mathcal{L}'^2 \\ c_1(l)\neq 0=c_2(l)}} Q_c E_c(x)\cdot\frac{1}{\tilde{c}_1(l)} = \sum_{\substack{c\in\mathcal{L}'^2 \\ c_2(l)\neq 0=c_1(l)}} Q_c E_c(x)\cdot\frac{1}{\tilde{c}_2(l)}$$

and thus the second and third summand cancel. Alternatively, we could use that the x-integration against E_{-Fl} removes all summands except those with

$$c_1 + c_2 = -Fl\,.$$

If this is the case, then, in particular, $c_1(l) + c_2(l) = -Fl(l) = 0$. Hence, terms with $c \in \mathcal{L}'^2$ such that $c_1(l) + c_2(l) \neq 0$ vanish under the x-integration.

The fourth sum can be shown to vanish by a symmetry consideration: If $(c_1, c_2) \in (\mathcal{L}')^2$ is a pair that satisfies $c_1(l) = -c_2(l) \neq 0$, then so is (c_2, c_1). Therefore, by swapping the indices and using $-1/\tilde{c}_2(l) = 1/\tilde{c}_1(l)$, we obtain

$$\sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1(l)=-c_2(l)\neq 0}} Q_c E_c(x) \frac{-1}{\tilde{c}_1(l)} = \sum_{\substack{c_2,c_1\in\mathcal{L}'\\ c_2(l)=-c_1(l)\neq 0}} Q_c E_c(x) \frac{-1}{\tilde{c}_2(l)} = \sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1(l)=-c_2(l)\neq 0}} Q_c E_c(x) \frac{1}{\tilde{c}_1(l)} = 0\,.$$

Overall, this gives the result

$$Q(x+\tau_2 l)Q(x+\tau_1\tau_2 l)\tau_2 \overset{\tau}{=} \sum_{\substack{c_1,c_2\in\mathcal{L}'\\ c_1(l)=0=c_2(l)}} Q_c E_c(x) \cdot \frac{1}{2}\,.$$

□

B.3 MATHEMATICA Algorithm

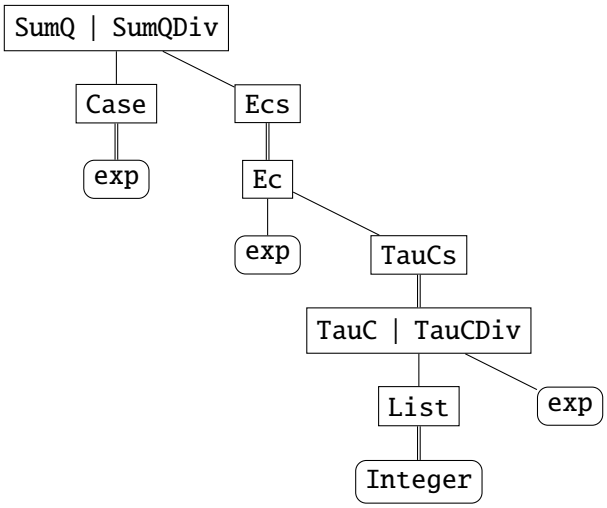
After illustrating the τ-integration and its two problems in the examples above we can now proceed to give a general algorithm to compute the τ-integrals. This is best done by explaining the MATHEMATICA structure used to describe those τ-integrals and the intermediate expressions used to compute them.

In this section we consider expressions more formally as a tree, where each subexpression has a *head* and *children*: Its topmost function and the arguments thereof, respectively. For example, the expression

$$1 + 2 + g(x)$$

has the head `Plus` (in MATHEMATICA notation) and the children 1, 2 and $g(x)$.

The expressions appearing while computing the τ-integrals are of the form given by the following tree, which we explain in more detail below.



Each node with a rectangular box `Head` represents the `Head` of the expression given by the corresponding subtree. The node (`Integer`) represents a single integer while the nodes (`exp`) represent unspecified subexpressions. Each `Head` has as many arguments as there are children in the graph. However, double lines indicate that the following expressions appear in varying number, but at least once. The node `TauC | TauCDiv` represents either `TauC` or `TauCDiv`. Definitions of the subtrees of the graph above are given in the remainder of this section.

We will explain the MATHEMATICA structure starting at the bottom of the tree given above. The integrals

$$\int_{[0,1]^\lambda} \tau^e \prod_{i=1}^{q} Q(x + l \cdot \tau^{b_i}, d_i)\, \mathrm{d}\tau$$

can be expressed without using the binary multiindices b explicitly.

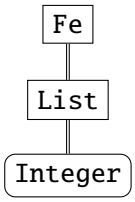
Definition B.10. If $e \in \mathbb{Z}^\lambda$ is a multiindex of length λ and $b \in (\mathrm{BM}^\lambda)^q$ in flag-form then the *fractured exponent* $f(e,b)$ is a tuple of tuples of the form

$$f(e,b) = \Big((e_1,\ldots,e_{h_1}),(e_{h_1+1},\ldots,e_{h_2}),\ldots,(e_{h_{q-1}+1},\ldots,e_\lambda)\Big)$$

such that each element $f_i \in f(e,b)$ is given by those elements of e for which

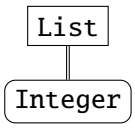
$b_i - b_{i+1}$ is equal to 1.

The fractured exponents shall be given the following MATHEMATICA structure:



This means that expressions with head `Fe` contain one or more `Lists` of integers.

On the other hand, multiindices e can be represented by the following tree:



Example B.11. The summand $Q(x + l\tau_2)Q(x + l\tau_1\tau_2) \cdot \tau_2 \cdot \frac{43}{32}\mathrm{i}|l|$ has the fractured exponent

$$\Big((0),(1)\Big)$$

and $Q(x + l\tau_2\tau_3\tau_4)Q(x + l\tau_1\tau_2\tau_3\tau_4, \{l,l,l,l\}) \cdot \tau_1^4\tau_2^5\tau_3^4\tau_4^3 \cdot \frac{1}{16}$ has the fractured exponent

$$\Big((4),(5,4,3)\Big).$$

It is clear that the fractured exponent $f(e,b)$ contains the same information as (e,b). Further, the τ-integral of any summand is independent of the order in each $f_i \in f(e,b)$. We may assume that f_i is an increasing multiindex. For example,

$$\Big((4),(3,4,5)\Big) \qquad \text{and} \qquad \Big((4),(5,4,3)\Big)$$

give the same integral.

Definition B.12. Given some multiindex $e \in \mathbb{Z}^\lambda$ and some b in flag-form we say that

$$p(b) \coloneqq (\#f(e,b)_1, \ldots, \#f(e,b)_q) \in \mathbb{Z}^q$$

is the *variable partition* corresponding to b. The multiindex e is called *partially increasing* with respect to a variable partition $p(b)$ if

$$f(e,b)_i \qquad \text{is an increasing multiindex for each } i \in \{1,\ldots,q\}.$$

Again, the variable partition $p(b)$ contains the same information as b. Also, the τ-integral does not depend on the order of the elements within each $f(e,b)_i$ and thus we can assume, without loss of generality, that the exponents e are partially increasing with respect to the given variable partition.

Remark B.13. Using partially increasing multiindices as exponents does *not* lead to a maximal number of τ-integrations: We can, loosely speaking, integrate up to the first τ-variable with index i such that

$$e_i = e_{i+1}\,.$$

Thus, we could perform more integrations if each part of the fractured exponent were arranged in such a way that its beginning is strictly increasing and of maximal length. For example, we could use

$$\big((1,2,3,1),(5)\big) \qquad \text{instead of} \qquad \big((1,1,2,3),(5)\big).$$

However, it will turn out that maximality in τ-integrations is not needed and, hence, we can continue with the simpler concept of partially increasing exponents.

Remark B.14 (Data).
Each τ-integrand

$$\tau^e \cdot Q(x + l\tau^{b_1}, d_1) \cdots Q(x + l\tau^{b_q}, d_q)$$

is encoded using three objects:

- The exponent e is assumed to be partially increasing and is stored as `List` of `Integers`.
- b is assumed to be in flag-form with $b_1 = \mathbb{1}$, i.e. there are no trivial τ-integrals. Instead of b we use its variable partition $p(b)$, which is also a `List` of `Integers`.
- The derivatives d are combined into the expression $c(d)$, see Definition B.2.

Definition B.15 (Exponents).
If we are given some expression

$$E_c(l\tau^{b_i}) \cdot \tau^e \cdot C = \mathrm{e}^{-\tilde{c}(l)\tau^{b_i}} \cdot \tau^e \cdot C$$

with some dual lattice vector $c \in \mathcal{L}'$, multiindex $e \in \mathbb{Z}^\lambda$ and a binary multiindex $b_i \in \mathrm{BM}^\lambda$ then we call

$\tilde{c}(l)$ the *E-exponent* and
e the *τ-exponent*.

In expressions $E_c(l\tau^b) \cdot C$ with $b \in (\mathrm{BM}^\lambda)^q$ in flag-form and C free of any functions E we call

$\tilde{c}_1(l)$ the *first E-exponent*.

The τ-integration consists of two algorithms that will be described in the remainder of this section.

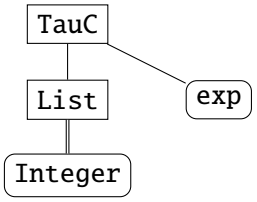
- ALGORITHM I (Integration) computes the $p(b)_h$ τ-integrals that correspond to the τ-variables that first appear in the h-th potential. This algorithm needs to know whether the first E-exponent of the current expression vanishes or not.
- ALGORITHM P (Partition) partitions the set $\mathcal{L}'^q$ such that after repeatedly applying ALGORITHM I and merging the first two E-exponents we can determine whether the new first E-exponent vanishes or not.

These two algorithms will be given below together with the MATHEMATICA structure required for the involved expressions.

Definition B.16 (τ-coefficient).
A *τ-coefficient* is a term of the form

$$\tau^e \cdot C\,, \qquad \text{where } C \text{ is independent of } \tau.$$

We give τ-coefficients the following MATHEMATICA structure:



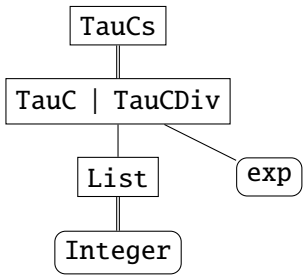
A τ-coefficient has the head `TauC` with two arguments: its exponent e and the coefficient C given by some expression `exp`.

A τ-coefficient that satisfies

$$e_1 < 0$$

shall be called *divergent*. Divergent τ-coefficients are given the head `TauCDiv`.

In the computation of wave invariants there are typically sums of divergent and nondivergent τ-coefficients. Such sums shall be called *τ-sums* and are given the head `TauCs`. Overall a sum of τ-coefficients has the following MATHEMATICA-structure:



We do not use the conventional `Plus` instead of `TauCs` because this would be automatically removed if there was only one summand. In this case the structure of our expression would change, which would require more complicated integration functions that recognize different structures. The same is true for `Ecs` below. Such expressions, where `TauCs` and `Ecs` have only one child, do appear in the computation of wave invariants.

So far we have only considered integrands with a single factor $E_{c_i}(l\tau^{b_i})$. But we have as many terms $E_{c_i}(l\tau^{b_i})$ as there are potentials in our integrand. The following ALGORITHM I expands Lemma B.7 to this case and integrates τ-variables.

ALGORITHM I. Let the $\mathcal{I}_t$, $\mathcal{I}_+(\tilde{c}_h(l))$ and $\mathcal{I}_-(\tilde{c}_h(l))$ denote linear functions that map τ-sums to τ-sums and are given by

$$\begin{aligned}
&\mathcal{I}_t(\tau^e) \coloneqq \tau^{\dagger e} \cdot \frac{1}{e_1+1}\,,\\
&\mathcal{I}_+(\tilde{c}_h(l))(\tau^e) \coloneqq \tau^{\dagger(e-(e_1+1))} \cdot e_1! \cdot \tilde{c}_h(l)^{-e_1-1} \qquad \text{and}\\
&\mathcal{I}_-(\tilde{c}_h(l))(\tau^e) \coloneqq \sum_{i=0}^{e_1} \tau^{\dagger(e+i-e_1-1))} \cdot \Big(-\frac{e_1!}{i!}\tilde{c}_h(l)^{i-e_1-1}\Big),
\end{aligned}$$

where it is assumed that $\tilde{c}_h(l) \neq 0$. With this definition we can reformulate Lemma B.7 and express the integral over τ_1 as

$$E_{c_h}(l\tau^{b_h}) \cdot \tau^e \overset{\tau}{=} \begin{cases} E_0(l\tau^{\dagger b_h}) \cdot \mathcal{I}_t(\tau^e) & \text{for } c_h(l) = 0 \text{ and for } c_h(l) \neq 0 \\ E_0(l\tau^{\dagger b_h}) \cdot \mathcal{I}_+(\tilde{c}_h(l))(\tau^e) + E_{c_h}(l\tau^{\dagger b_h}) \cdot \mathcal{I}_-(\tilde{c}_h(l))(\tau^e)\,, \end{cases}$$

where it is assumed that $b_h = \mathbb{1} \in \mathrm{BM}^\lambda$. $\mathcal{I}_t$ is called the *trivial integration* while the second line using $\mathcal{I}_+(\tilde{c}_h(l))$ and $\mathcal{I}_-(\tilde{c}_h(l))$ is called *nontrivial integration*.

If we want to compute integrands of the form

$$E_{c_h}(l\tau^{b_h})E_{c_{h+1}}(l\tau^{b_{h+1}}) \cdots E_{c_q}(l\tau^{b_q}) \cdot \tau^e$$

we can apply Lemma B.7 and factors of the form $E_{c_k}(l\tau^{b_k})$ with $b_{k,1} = 0$ remain unchanged under such an integration. For the sake of consistency of the exponentials we need to drop the first indices in b_k, even though they are zero anyway. We replace

$$b_k \qquad \text{by} \qquad \dagger\, b_k\,.$$

Therefore,

$$E_c^h(l\tau^b)\cdot\tau^e = E_{c_h}(l\tau^{b_h})E_{c_{h+1}}(l\tau^{b_{h+1}})\cdots E_{c_q}(l\tau^{b_q})\cdot\tau^e$$
$$\overset{\tau}{=}\begin{cases} E_0(l\tau^{\dagger b_h})\cdot\mathcal{I}_t(\tau^e)\cdot E_c^{h+1}(l\tau^{\dagger b}) & \text{for } c_h(l)=0 \\ E_0(l\tau^{\dagger b_h})\cdot\mathcal{I}_+(\tilde{c}_h(l))(\tau^e)\cdot E_c^{h+1}(l\tau^{\dagger b}) & \\ \qquad +E_{c_h}(l\tau^{\dagger b_h})\cdot\mathcal{I}_-(\tilde{c}_h(l))(\tau^e)\cdot E_c^{h+1}(l\tau^{\dagger b}) & \text{for } c_h(l)\neq 0. \end{cases}$$

The τ-coefficients obtained from this rule have different exponents of the same length. This rule can be applied repeatedly as long as $e_1 \geq 0$ and $b_{h+1,1} = 0$. The condition $b_{h+1,1} = 0$ is satisfied for $p(b)_h$ integrations and thus the variable partition gives us the number of repetitions of ALGORITHM I.

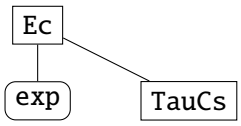
Finally, we define ALGORITHM I to have no effect on divergent τ-coefficients.

ALGORITHM I shows that the sums of τ-coefficients are multiplied by factors of the form $E_{c_i}(l\tau^{b_i})$, where $c_i \in \mathcal{L}'$ and b_i is a binary multiindex. It should be noted that the information contained within $E_c^{h+1}(l\tau^{\dagger b})$ is already contained in the variable partition $p(b)$ (provided some $c \in \mathcal{L}'^q$ is fixed) and for this reason those terms are excluded from the MATHEMATICA structure.

Definition B.17. If C is some τ-sum, $c_h \in \mathcal{L}'$ is a dual lattices vector and $b_h = \mathbb{1} \in \mathrm{BM}^\lambda$ then

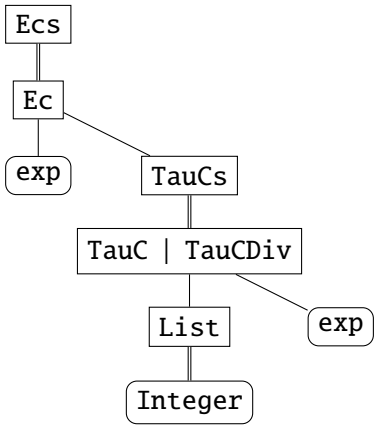
$$E_{c_h}(l\tau^{b_h})\cdot C$$

is given the following MATHEMATICA structure:



where the children of `TauCs` are omitted. `TauCs` contains C and (`exp`) is an expression describing c_h. The dual lattice vector c_h is always applied to $l\tau^{b_h}$ and the information provided by b_h is contained within the variable partition. Hence, we do not need to store the lattice vector $l \in \mathcal{L}\backslash\{0\}$ nor the binary multiindex b_h.

Sums of such terms $E_c(l\tau^{b_h})\cdot C$ are given the head `Ecs`. Overall this gives the following structure:



We can apply Algorithm I to such structures and it will return such structures as long as $b_{h+1,1} = 0$ or, equivalently, for $p(b)_h$ iterations. (Divergent τ-coefficients are not affected by Algorithm I.)

Now, let us assume that we have applied this algorithm until we have

$$b_{h+1,1} = 1 \qquad \text{or equivalently} \qquad b_h = b_{h+1}\,.$$

Then we can no longer ignore the factor $E_{c_{h+1}}(l\tau^{b_{h+1}})$ and we have

$$E_0(l\tau^{b_h}) \cdot E_{c_{h+1}}(l\tau^{b_{h+1}}) = E_{c_{h+1}}(l\tau^{b_{h+1}}) \qquad \text{and}$$
$$E_{c_h}(l\tau^{b_h}) \cdot E_{c_{h+1}}(l\tau^{b_{h+1}}) = E_{c_h+c_{h+1}}(l\tau^{b_{h+1}})\,.$$

To continue with the τ-integration we need to distinguish whether the E-exponents vanish or not. For the first line we have to consider the cases $c_{h+1}(l) = 0$ and $c_{h+1}(l) \neq 0$ and for the second line the cases $c_{h+1}(l) = 0$, $(c_h + c_{h+1})(l) = 0$ and $(c_h + c_{h+1})(l) \neq 0$. To this end we will partition the set $\mathcal{L}'^q$ into subsets called *cases* that are constructed from this distinction. Using those sets will allow us to continue the τ-integration using Algorithm I.

The definition of the *cases* requires some use of *formal* notation. If we write, say, $\mathfrak{c}_i \equiv \sum \pm c_j$ in the following definition, then this means that $\mathfrak{c}_i$ is a formula given by the string of symbols on the right hand side of this equivalence.

Definition B.18 (Case).
For $l \in \mathcal{L}\backslash\{0\}$ an *unintegrated case* is a subset

$$l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x \subset (\mathcal{L}')^q$$

where in the place of $\mathfrak{c}_i$ we can either have 0 or c_i or some sum $\sum \pm c_j$ with $j < i$. For any tuple of dual lattice vectors $c \in l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x$ the following must hold:

- If $\mathfrak{c}_i \equiv 0$, then $c_i(l) = 0$.

- If $\mathfrak{c}_i \equiv c_i$, then for all $1 \leq s \leq i$ the following sum is nonvanishing $c_s(l) + \cdots + c_i(l) \neq 0$.
- If $\mathfrak{c}_i \equiv \sum \pm c_j$, then $c_i(l) = \sum \pm c_j(l)$.

The subscript x refers to the (unperformed) x-integration. Eventually only those terms remain that do not vanish under the x-integration $\langle\,.\,, E_{-Fl}\rangle$. Since the terms with an A_x^{D}-dependence cancel in the wave invariants, see Lemma 4.41, only those subsets of the cases will remain that also satisfy $c_1 + \cdots + c_q = -Fl$. A *case* $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$ is the subset of the unintegrated case $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x$ where each element c additionally satisfies $c_1 + \cdots + c_q = -Fl$.

Given some unintegrated case $\mathfrak{c}$ or some tuple of dual lattice vectors $c \in \mathcal{L}'^h$ of length h the i-th *end* of $\mathfrak{c}$ or c is defined as

$$\mathfrak{e}_i\mathfrak{c} \coloneqq \sum_{j=i}^{h} \mathfrak{c}_j \qquad \text{and, analogously,} \qquad \mathfrak{e}_i c \coloneqq \sum_{j=i}^{h} c_j\,.$$

Let $C_l(h)$ denote the set of all possible unintegrated cases of length h for some lattice vector $l \in \mathcal{L}$. More precisely,

$$\begin{aligned} C_l(1) &\coloneqq \{l[0]_x,\, l[c_1]_x\} \qquad \text{and} \\ C_l(h+1) &\coloneqq \bigcup_{\mathfrak{c} \in C_l(h)} \mathrm{nc}(\mathfrak{c})\,, \end{aligned}$$

where the function $\mathrm{nc}(\mathfrak{c})$ generates new cases based on the unintegrated case $\mathfrak{c}$ as follows.

$$\begin{aligned} \mathrm{nc}(\mathfrak{c}) \coloneqq \Big\{ & l[\mathfrak{c}_1, \ldots, \mathfrak{c}_h, 0]_x,\, l[\mathfrak{c}_1, \ldots, \mathfrak{c}_h, c_{h+1}]_x \Big\} \\ & \cup \{ l[\mathfrak{c}_1, \ldots, \mathfrak{c}_h, -\mathfrak{e}_i\mathfrak{c}]_x \mid i = 1, \ldots, h \}\,. \end{aligned}$$

Further, we define

$$C_l^q(h) \coloneqq \left\{ \mathfrak{c} \times \mathcal{L}'^{q-h} \mid \mathfrak{c} \in C_l(h) \right\}.$$

Elements of $C_l(h)$ are subsets of $\mathcal{L}'^h$, while elements of $C_l^q(h)$ are subsets of the larger $\mathcal{L}'^q$. For $c \in \mathfrak{c} \in C_l^q(h)$ any *end* of c refers only to the part of c that corresponds to $C_l(h)$, i.e.

$$\mathfrak{e}_i c \coloneqq \sum_{j=i}^{h} c_j\,.$$

It is clear that each $C_l^q(h)$ is a partition of $\mathcal{L}'^q$. In particular, $C_l(q) = C_l^q(q)$ is a partition of $\mathcal{L}'^q$.

Example B.19. We have

$$\mathrm{nc}(l[0]_x) = \{l[0,0]_x,\, l[0,c_2]_x\} \quad \text{and} \quad \mathrm{nc}(l[c_1]_x) = \{l[c_1,0]_x,\, l[c_1,c_2]_x,\, l[c_1,-c_1]_x\}$$

and therefore

$$C_l(2) = \{l[0,0]_x,\, l[0,c_2]_x,\, l[c_1,0]_x,\, l[c_1,c_2]_x,\, l[c_1,-c_1]_x\}\,.$$

While the entries of the *cases* are formal we still assume that the usual simplification rules are applied and that the *ends* of the cases are minimal. For example,

$$\mathfrak{e}_1 l[c_1,-c_1] \equiv c_1 - c_1 \equiv 0 \qquad \text{and} \qquad -\mathfrak{e}_2 l[c_1,-c_1] \equiv -(-c_1) \equiv c_1\,.$$

Thus we have

$$\begin{aligned} C_l(3) = \Big\{ & l[0,0,0]_x,\, l[0,0,c_3]_x, \\ & l[0,c_2,0]_x,\, l[0,c_2,c_3]_x,\, l[0,c_2,-c_2]_x, \\ & l[c_1,0,0]_x,\, l[c_1,0,c_3]_x,\, l[c_1,0,-c_1]_x, \\ & l[c_1,c_2,0]_x,\, l[c_1,c_2,c_3]_x,\, l[c_1,c_2,-c_2]_x,\, l[c_1,c_2,-c_1-c_2]_x, \\ & l[c_1,-c_1,0]_x,\, l[c_1,-c_1,c_3]_x,\, l[c_1,-c_1,c_1]_x \Big\}\,. \end{aligned}$$

Lemma B.20. The unintegrated cases $\mathfrak{c} \in C_l(h)$ are constructed in such a way that for all indices $i \in \{1,\dots,h\}$

$$\mathfrak{e}_i\mathfrak{c} \equiv 0 \qquad \text{if and only if} \qquad \forall_{c\in\mathfrak{c}} : \mathfrak{e}_i c(l) = 0\,.$$

Proof. If $\mathfrak{c} = l[\mathfrak{c}_1,\dots,\mathfrak{c}_h]_x \in C_l(h)$ is an unintegrated case of length h let $\mathfrak{c}_{\le j} \coloneqq l[\mathfrak{c}_1,\dots,\mathfrak{c}_j]_x \in C_l(j)$ denote the unintegrated subcase given by the first j entries of $\mathfrak{c}$. Analogously, $c_{\le j} \coloneqq (c_1,\dots,c_j)$. The claim holds for $h = 1$ because

$$C_l(1) = \{l[0]_x, l[c_1]_x\}\,.$$

So if $\mathfrak{c} = l[0]_x$ then $\mathfrak{e}_1\mathfrak{c} \equiv 0$ and for all $c \in \mathfrak{c}$ we have $\mathfrak{e}_1 c(l) = 0$. If $\mathfrak{c} \equiv l[c_1]_x$ then $\mathfrak{e}_1\mathfrak{c} \not\equiv 0$ and $\mathfrak{e}_1 c(l) \neq 0$ for all $c \in \mathfrak{c}$.

Let us now inductively assume that the Lemma holds for all unintegrated cases with length less than h. If $\mathfrak{c} \in C_l(h)$ with $h > 1$ then there are three cases to distinguish: $\mathfrak{c}_h \equiv 0$, $\mathfrak{c}_h \equiv c_h$ and $\mathfrak{c}_h \equiv -\mathfrak{e}_j\mathfrak{c}_{\le(h-1)}$ for some $j \in \{1,\dots,h-1\}$.

If $\mathfrak{c}_h \equiv 0$ and $i < h$ then $\mathfrak{e}_i\mathfrak{c} \equiv \mathfrak{e}_i\mathfrak{c}_{\le(h-1)} \equiv 0$ exactly if $\mathfrak{e}_i c(l) = \mathfrak{e}_i c_{\le(h-1)}(l) = 0$ for all $c \in \mathfrak{c}$ by induction. If $\mathfrak{c}_h \equiv c_h$ then $\mathfrak{e}_i\mathfrak{c} \not\equiv 0$ and $\mathfrak{e}_i c(l) \neq 0$ for all all $i \in \{1,\dots,h\}$ and $c \in \mathfrak{c}$.

If, now, $\mathfrak{c}_h \equiv -\mathfrak{e}_j\mathfrak{c}_{\le(h-1)}$ we first assume that $i < j$. Then,

$$\mathfrak{e}_i\mathfrak{c} \equiv \mathfrak{e}_i\mathfrak{c}_{\le(h-1)} - \mathfrak{e}_j\mathfrak{c}_{\le(h-1)} \equiv \mathfrak{c}_i + \cdots + \mathfrak{c}_{j-1} \equiv \mathfrak{e}_i\mathfrak{c}_{\le(j-1)}\,.$$

By induction, $\mathfrak{e}_i\mathfrak{c} \equiv \mathfrak{e}_i\mathfrak{c}_{\le(j-1)} \equiv 0$ exactly if $\mathfrak{e}_i c(l) = \mathfrak{e}_i c_{\le(j-1)}(l) = 0$ for all $c \in \mathfrak{c}$.

If $i > j$ then

$$\mathfrak{e}_i\mathfrak{c} \equiv \mathfrak{e}_i\mathfrak{c}_{\leq(h-1)} - \mathfrak{e}_j\mathfrak{c}_{\leq(h-1)} \equiv -(\mathfrak{c}_j + \cdots + \mathfrak{c}_{i-1}) \equiv -\mathfrak{e}_j\mathfrak{c}_{\leq(i-1)}$$

and the claim follows again.

If $i = j$ then $\mathfrak{e}_i\mathfrak{c} \equiv \mathfrak{e}_i\mathfrak{c}_{\leq(h-1)} - \mathfrak{e}_j\mathfrak{c}_{\leq(h-1)} \equiv 0$ and, analogously, $\mathfrak{e}_i c(l) = 0$ for all $c \in \mathfrak{c}$. This concludes the induction. □

The definition of cases allows us to describe ALGORITHM P. But before doing that we introduce an abbreviation. We have already seen in the examples that the terms $Q_c E_c(x)$ are unaffected by the τ-integration and that they can be omitted.

Definition B.21 (Q-sum).
If $C \subset \mathcal{L}'^q$ is some set of tuples of dual lattice vectors we write

$$\sum_{c\in C}^{Q} f(c) \coloneqq \sum_{c\in C} Q_c E_c(x) \cdot f(c)\,.$$

If this set C happens to be an integrated case, $C = l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$, we assume that the x-integration has removed the term $E_c(x)$ from the expression and it is understood that

$$\sum_{c\in l[\mathfrak{c}_1,\ldots,\mathfrak{c}_q]}^{Q} f(c) \coloneqq \sum_{c\in l[\mathfrak{c}_1,\ldots,\mathfrak{c}_q]} Q_c f(c)\,.$$

Both abbreviations shall be called *Q-sums*.

Remark B.22. Not every unintegrated case $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x$ is integrable (with respect to x): The definition of a case requires that we have for all $c \in l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$ that

$$c_1 + \cdots + c_q = -Fl \quad \text{and thus} \quad (c_1 + \cdots + c_q)(l) = -Fl(l) = -F(l,l) = 0\,.$$

If we have an unintegrated case $l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x$ with $\mathfrak{c}_1 + \cdots + \mathfrak{c}_q \not\equiv 0$ then, by Lemma B.20,

$$l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q] = \emptyset\,.$$

In particular, corresponding Q-sums vanish upon x-integration:

$$\langle \sum_{c\in l[\mathfrak{c}_1,\ldots,\mathfrak{c}_q]_x}^{Q} f(c), E_{Fl}\rangle = \sum_{c\in l[\mathfrak{c}_1,\ldots,\mathfrak{c}_q]}^{Q} f(c) = 0\,,$$

provided f is free of x.

Algorithm P. Before introducing the transition from the h-th potential to the $(h+1)$-th potential let us first study the effect of Algorithm I on certain expressions. Fix some unintegrated case $\mathfrak{c} \in C_l(h)$ and consider the following expression

$$E_0(l\tau^{B_h}) \cdot C_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c}(l\tau^{B_h}) \cdot C_{i,\mathfrak{c},c}(\tau) \qquad \text{with } c \in \mathfrak{c},$$

where $C_{i,\mathfrak{c},c}(\tau)$ are τ-sums that depend on the index i, the unintegrated case $\mathfrak{c}$, $c \in \mathfrak{c}$ and τ. We assume that the $C_{i,\mathfrak{c},c}(\tau)$ are given by previous τ-integrations. Also, B is a tuple of binary multiindices in flag-form, obtained from b by dropping indices (again in previous integrations). Lemma B.20 tells us that whether the E-exponents vanish or not depends only on the case $\mathfrak{c}$. Thus, we can decide for each summand if we have to apply the trivial or the nontrivial integration and this decision is then correct for all $c \in \mathfrak{c}$. After computing those integrations $p(b)_h$ times we obtain again an expression of the form

$$E_0(l\tau^{\dagger^{p(b)_h} B_h}) \cdot C'_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c}(l\tau^{\dagger^{p(b)_h} B_h}) \cdot C'_{i,\mathfrak{c},c}(\tau)$$

with new τ-sums $C'_{i,\mathfrak{c},c}(\tau)$.

Let us assume inductively that after integrating the τ-variables of the first h potentials, i.e. the first $H := p(b)_1 + \cdots + p(b)_h$ τ-variables, we obtain a sum over all unintegrated cases $C_l^q(h)$ of the following form:

$$\sum_{c \in \mathcal{L}'^q}^{Q} E_{c_1}(l\tau^{b_1}) \cdots E_{c_q}(l\tau^{b_q}) \cdot \tau^e$$

$$\stackrel{\tau}{=} \sum_{\mathfrak{c} \in C_l^q(h)} \sum_{c \in \mathfrak{c}}^{Q} \Big(E_0(l\tau^{\dagger^H b_h}) \cdot C_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c}(l\tau^{\dagger^H b_h}) \cdot C_{i,\mathfrak{c},c}(\tau) \Big) \cdot E_c^{h+1}(l\tau^{\dagger^H b}) \,.$$

By the definition of the variable partition $p(b)$

$$\dagger^H b_h = \dagger^H b_{h+1}$$

and therefore, with $B := \dagger^H b$,

$$\sum_{\mathfrak{c} \in C_l^q(h)} \sum_{c \in \mathfrak{c}}^{Q} \Big(E_0(l\tau^{B_h}) \cdot C_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c}(l\tau^{B_h}) \cdot C_{i,\mathfrak{c},c}(\tau) \Big) \cdot E_c^{h+1}(l\tau^{B})$$

$$= \sum_{\mathfrak{c} \in C_l^q(h)} \sum_{c \in \mathfrak{c}}^{Q}$$

$$\Big(E_{c_{h+1}}(l\tau^{B_{h+1}}) \cdot C_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c + c_{h+1}}(l\tau^{B_{h+1}}) \cdot C_{i,\mathfrak{c},c}(\tau) \Big) \cdot E_c^{h+2}(l\tau^{B}) \,.$$

To be able to reapply Lemma B.20 and ALGORITHM I we want to partition the sum over $c_{h+1} \in \mathcal{L}'$ such that we can easily decide whether the first E-exponents vanish or not. That leads us to differentiate between

- $c_{h+1}(l) = 0$,
- $\mathfrak{e}_i c + c_{h+1} = 0$ for $i \in \{1, \dots, h\}$ and
- neither of those terms vanishes.

This is exactly how the unintegrated cases are defined; for a fixed unintegrated case $\mathfrak{c} \in C_l^q(h)$ the desired partition is given by the new cases $\mathtt{nc}(\mathfrak{c})$. Therefore, our expression can be written as

$$\sum_{\mathfrak{c} \in C_l^q(h)} \sum_{c \in \mathfrak{c}}^{Q} \Big(E_0(l\tau^{B_h}) \cdot C_{0,\mathfrak{c},c}(\tau) + \sum_{i=1}^{h} E_{\mathfrak{e}_i c}(l\tau^{B_h}) \cdot C_{i,\mathfrak{c},c}(\tau) \Big) \cdot E_c^{h+1}(l\tau^B)$$

$$= \sum_{\mathfrak{c} \in C_l^q(h+1)} \sum_{c \in \mathfrak{c}}^{Q} \Big(E_0(l\tau^{B_{h+1}}) \cdot 0 + \sum_{i=1}^{h+1} E_{\mathfrak{e}_i c}(l\tau^{B_{h+1}}) \cdot C_{i,\mathfrak{c},c}(\tau) \Big) \cdot E_c^{h+2}(l\tau^B)$$

with $C_{h+1,\mathfrak{c},c}(\tau) \coloneqq C_{0,\mathfrak{c},c}(\tau)$. This expression satisfies $B_{h+2,1} = 0$ and for each unintegrated case $\mathfrak{c}$ and its Q-sum we can determine which E_c-terms, $c \in \mathfrak{c}$, require the trivial and which E_c-terms require the nontrivial integration. Hence, we can apply ALGORITHM I to its inner sum.

We repeat this process of generating new cases via ALGORITHM P and then applying ALGORITHM I. The variable partition determines how often each algorithm has to be used: ALGORITHM P has to be applied $q = \#p(b)$ times and ALGORITHM I has to be applied $p(b)_h$ times at each step. After $p(b)_1 + \cdots + p(b)_q$ integrations, all τ-variables have been integrated.

So far we have not given a basis for this induction and we have not included the derivatives in this computation. We use

$$C_l^q(0) = \{\mathcal{L}'^q\}$$

and start with

$$Q(x + l\tau^{b_1}, d_1) \cdots Q(x + l\tau^{b_q}, d_q) \cdot \tau^e = \sum_{\mathfrak{c} \in C_l^q(0)} \sum_{c \in \mathfrak{c}}^{Q} E_c(l\tau^b) \cdot \Big(\tau^e \cdot (-\tilde{c})(d) \Big),$$

where $(-\tilde{c})(d)$ is given in Definition B.2.

Remark B.23. We have been somewhat vague as what to do when the τ-exponent e is not strictly increasing. If e is not strictly increasing then we use ALGORITHM I and ALGORITHM P until divergent τ-coefficients appear. We then

leave those divergent τ-coefficients unchanged and continue to integrate the nondivergent τ-coefficients.

Remark B.24. Further, the sum over the ends of some (integrated or unintegrated) case $\mathfrak{c}$

$$\sum_{c\in\mathfrak{c}}^{Q}\Big(E_0(l\tau^{b_h})\cdot C_{0,\mathfrak{c}}(\tau)+\sum_{i=1}^{h}E_{\mathfrak{e}_i c}(l\tau^{b_h})\cdot C_{i,\mathfrak{c}}(\tau)\Big),$$

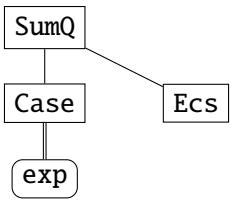
and its τ-sums $C_{i,\mathfrak{c},c}(\tau)$ are not uniquely determined, because ends with different indices i may be (formally) equal. For example, if $\mathfrak{c}\equiv l[c_1,-c_1,c_1,-c_1]$ then

$$\mathfrak{e}_1 l[c_1,-c_1,c_1,-c_1]\equiv 0\equiv \mathfrak{e}_3 l[c_1,-c_1,c_1,-c_1]\,.$$

We take a minimalistic approach and assume that in such cases there is only one summand and its τ-sum is the sum of the individual τ-summands. For the case $\mathfrak{c}=l[c_1,-c_1,c_1,-c_1]$

$$\sum_{c\in\mathfrak{c}}^{Q}\Big(E_0(l\tau^{b_H})\cdot(C_{0,\mathfrak{c},c}+C_{1,\mathfrak{c},c}+C_{3,\mathfrak{c},c})(\tau)+E_{-c_1}(l\tau^{b_H})\cdot(C_{2,\mathfrak{c},c}+C_{4,\mathfrak{c},c})(\tau)\Big).$$

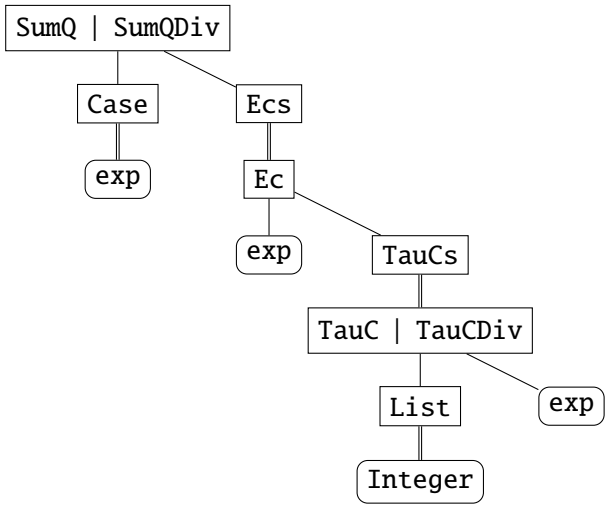
Finally, we need to extend our MATHEMATICA structure to encompass the sums over the unintegrated cases. The sum $\sum_{\mathfrak{c}\in\mathcal{C}_l^q(h)}$ will use the conventional summation and requires no special `Head`. However, the sum $\sum_{c\in\mathfrak{c}}^{Q}$ needs the case $\mathfrak{c}$ as an argument. The sums $\sum_{c\in\mathfrak{c}}^{Q}f(c)$ will be represented by the following structure:



`Ecs` contains $f(c)$ and its children are omitted here. We will always use the letter c for the indices in such sums and for this reason there is no need to specify this index. The children of `Case` are expressions that correspond to the formal description of the case in question.

Finally, it is beneficial to split Q-sums into two sums, where one sum contains only nondivergent τ-coefficients while the other contains only divergent τ-coefficients. We use the head `SumQDiv` for the latter sums.

Overall, we therefore need the following MATHEMATICA structure:



The implementation of Algorithm I and Algorithm P into Mathematica code is given in Appendix D.

B.4 Symmetry

After computing the τ-integrals the resulting wave invariants are very large expressions and it is necessary and possible to apply simplifications to them. One of those simplifications is discussed here: using symmetries in the c-variables.

Example B.25. Consider the Q-sum

$$\sum_{c\in l[c_1,-c_1]_x}^{Q} f(c_1,c_2)\,.$$

Per definitionem $\mathfrak{c} := l[c_1,-c_1]_x = \big\{c \in \mathcal{L}'^2 \mid c_1(l) \neq 0 \text{ and } c_2(l) = -c_1(l)\big\}$. Thus, if $c = (c_1,c_2) \in \mathfrak{c}$ then the permuted $\pi_{(2,1)}c := (c_2,c_1)$ is also an element of $\mathfrak{c}$ and the permutation $\pi_{(2,1)}\colon \mathfrak{c} \to \mathfrak{c}$ is a bijection. Since $Q_cE_c = Q_{\pi_{(2,1)}c}E_{\pi_{(2,1)}c}$, it follows that

$$\begin{aligned}\sum_{c\in l[c_1,-c_1]_x}^{Q} f(c_1,c_2) &= \sum_{c\in l[c_1,-c_1]_x}^{Q} \frac{1}{2}\Big(f(c)+f(\pi_{(2,1)}c)\Big)\\ &= \sum_{c\in l[c_1,-c_1]_x}^{Q} \frac{1}{2}\Big(f(c_1,c_2)+f(c_2,c_1)\Big).\end{aligned}$$

If, say, $f(c_1,c_2) = 1/\tilde{c}_1(l)$ then the permutation $\pi_{(2,1)}$ and the definition of the case $l[c_1,-c_1]$ yield

$$\sum_{c\in l[c_1,-c_1]_x}^{Q} \frac{1}{\tilde{c}_1(l)} = \sum_{c\in l[c_1,-c_1]_x}^{Q} \frac{1}{2}\Big(\frac{1}{\tilde{c}_1(l)}+\frac{1}{\tilde{c}_2(l)}\Big) = \sum_{c\in l[c_1,-c_1]_x}^{Q} \frac{1}{2}\Big(\frac{1}{\tilde{c}_1(l)}-\frac{1}{\tilde{c}_1(l)}\Big) = 0\,.$$

Of course, this simplification requires that the permutation $\pi_{(2,1)}$ is a bijection of the (unintegrated) case $\mathfrak{c}$.

Definition B.26. Let σ denote a permutation of $\{1,\dots,q\}$ and $\mathfrak{c} \subset \mathcal{L}'^q$. We call

$$\pi_\sigma \colon \mathcal{L}'^q \to \mathcal{L}'^q \qquad \text{with } \pi_\sigma c := (c_{\sigma(1)},\dots,c_{\sigma(q)})$$

an *acceptable permutation* with respect to $\mathfrak{c}$ if

$$\pi_\sigma(\mathfrak{c}) = \mathfrak{c}$$

If a permutation π_σ is acceptable then it can be used to reformulate the Q-sum of the corresponding (unintegrated) case. In the following we construct an algorithm that, given some case $\mathfrak{c}$, returns the acceptable permutations.

Lemma B.27. If $\mathfrak{c} \subset \mathcal{L}'^q$ and π_σ is a permutation with $\pi_\sigma(\mathfrak{c}) \subset \mathfrak{c}$ then

$$\pi_\sigma(\mathfrak{c}) = \mathfrak{c}\,.$$

In other words, if $\mathfrak{c}$ is some (unintegrated) case and $\pi_\sigma(c) \in \mathfrak{c}$ for all $c \in \mathfrak{c}$ then π_σ is acceptable.

Proof. $\pi_\sigma \colon \mathcal{L}'^q \to \mathcal{L}'^q$ is bijective with inverse $\pi_{\sigma^{-1}}$. In particular, $\pi_\sigma \colon \mathfrak{c} \to \mathfrak{c}$ is injective. If $\|.\|$ is any norm of $\mathbb{R}^{n'}$ set $\|c\| := \|c_1\| + \ldots + \|c_q\|$ and $\mathfrak{c}_K := \{c \in \mathfrak{c} \mid \|c\| < K\}$. Since $\|\pi_\sigma c\| = \|c\|$ we have

$$\pi_\sigma(\mathfrak{c}_K) \subset \mathfrak{c}_K$$

and because $\mathfrak{c}_K$ is finite for every $K > 0$ and π_σ injective we have

$$\pi_\sigma(\mathfrak{c}_K) = \mathfrak{c}_K\,.$$

Therefore, $\pi_\sigma \colon \mathfrak{c} \to \mathfrak{c}$ is surjective and $\pi_\sigma(\mathfrak{c}) = \mathfrak{c}$. □

Example B.28. Not every permutation is acceptable. In the unintegrated case $\mathfrak{c} = l[c_1, -c_1, c_1]_x$ the permutations

$$(1,2,3) \quad \text{and} \quad (3,2,1)$$

are acceptable while the permutations

$$(1,3,2),\ (2,1,3),\ (2,3,1) \quad \text{and} \quad (3,1,2) \qquad \text{are not.}$$

Let $\mathfrak{c} \coloneqq l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]_x$ denote some fixed unintegrated case.

It is clear that any permutation that is acceptable with respect to $\mathfrak{c}$ can never exchange parts corresponding to $\mathfrak{c}_i \equiv 0$ with those that correspond to $\mathfrak{c}_i \not\equiv 0$. On the other hand, all components with $\mathfrak{c}_i \equiv 0$ can be permuted. Thus, the acceptable permutations are the product of all permutations of the zero components with the acceptable permutations of the remaining subcase. Without loss of generality, we assume that all entries of $\mathfrak{c}$ are nonzero, $\mathfrak{c}_i \not\equiv 0$.

To test whether a given permutation π_σ is acceptable with respect to the unintegrated case $\mathfrak{c}$ we describe the case using two sets of (in)equations. On the one hand, we take the set of all formal sums of $\mathfrak{c}$ that cannot be zero if $c \in \mathfrak{c}$. This set is given by

$$\texttt{SumsN0}(\mathfrak{c}) \coloneqq \left\{ \mathfrak{e}_j c_{\leq i} \equiv c_j + \ldots + c_i \mid 1 \leq j < i \leq q \quad \text{and} \quad \mathfrak{c}_i \equiv c_i \right\},$$

where we exclude sums of length one as those are trivially nonzero by assumption.

Definition B.29. Let $\mathfrak{c} = l[\mathfrak{c}_1, \ldots, \mathfrak{c}_q]$ denote some case. If $s(c_1, \ldots, c_q) = \sum_{i \in I} c_i$ is a formal sum, we define the *substitution by the case* $\mathfrak{c}$ as

$$s \mathbin{/.} \mathfrak{c} \coloneqq s(\mathfrak{c}_1, \ldots, \mathfrak{c}_q).$$

We call a formal sum *zero* if $s \equiv 0$. A formal sum is called *vanishing* if $s(c) = 0$ and *never vanishing* if $s(c) \neq 0$ for all $c \in \mathfrak{c}$.

It is important to note that while a formal sum is zero if and only if it is vanishing, there are nonzero sums that are not never vanishing. If formally $s \not\equiv 0$ there may still be elements $c \in \mathfrak{c}$ with $s(c) = 0$.

The set $\texttt{SumsN0}(\mathfrak{c})$ contains only those never vanishing formal sums that follow immediately from the definition of the unintegrated cases. Other formal sums that may also be never vanishing are not included.

On the other hand, we take the set of all formal sums that must vanish if we apply the substitutions for the $\mathfrak{c}_i$ prescribed by the unintegrated case $\mathfrak{c}$:

$$\texttt{Sums0}(\mathfrak{c}) \coloneqq \{ \Sigma_{i \in I} c_i \mid I \subset \{1 \ldots, q\} \quad \text{with} \quad \Sigma_{i \in I} c_i \mathbin{/.} \mathfrak{c} \equiv 0 \}.$$

Some $c \in \mathcal{L}'^q$ is an element of the unintegrated case $\mathfrak{c}$ exactly if the formal sums in the first set evaluate to nonzero and the formal sums in the second set evaluate to zero when evaluated for c. We want to test this for $\pi_\sigma(c)$ provided $c \in \mathfrak{c}$. Consider two substitutions performed upon a formal sum $\Sigma_{i \in I} c_i$:

(1) The substitution by the permutation acts upon a formal sum by permuting its summands.

$$\Sigma_{i \in I} c_i \mathbin{/.} \pi_\sigma \coloneqq \Sigma_{i \in I} c_{\pi_\sigma i}$$

(2) The (unintegrated) case itself acts upon a formal sum, $\Sigma_{i\in I}\, c_i$ /. $\mathfrak{c}$, by replacing all c_i by $\Sigma \pm c_j$ if $\mathfrak{c}_i \equiv \Sigma \pm c_j$.

Heuristically, the substitution by the permutation incorporates the effect of π_σ while the second substitution includes the knowledge about c gained from the assumption that $c \in \mathfrak{c}$.

Now, to test whether π_σ is acceptable we first apply the corresponding substitution to both the vanishing and the nonvanishing sums. For the vanishing sums we only need to apply the substitutions given by the case $\mathfrak{c}$ and check whether the resulting formal sums are zero. Is

$$\texttt{Sums0}(\mathfrak{c})\ /.\ \pi_\sigma\ /.\ \mathfrak{c} = \{0\}\,?$$

The consideration of the nonvanishing sums is not so simple, however.

Example B.30. Consider the unintegrated case $\mathfrak{c} \coloneqq l[c_1, c_2, c_3]_x$ and the permutation $\sigma = (1,3,2)$. There are no formal sums that vanish, so we only need to be concerned with the never vanishing formal sums

$$\texttt{SumsN0}(\mathfrak{c}) = \{c_1 + c_2,\ c_2 + c_3,\ c_1 + c_2 + c_3\}\,.$$

Applying the permutation gives

$$\texttt{SumsN0}(\mathfrak{c})\ /.\ \pi_\sigma = \{c_1 + c_3,\ c_3 + c_2,\ c_1 + c_3 + c_2\}$$

and all of those sums are formally nonzero. However,

$$c = (c_1, c_2, c_3) \qquad \text{with} \qquad c_1(l) = 1, \quad c_2(l) = 2, \quad c_3(l) = -1$$

is an element of $\mathfrak{c}$ with

$$c_1(l) + c_3(l) = 0 \qquad \text{and thus} \qquad \pi_\sigma c \notin \mathfrak{c}\,.$$

In particular, the permutation corresponding to $\sigma = (1,3,2)$ maps never vanishing formal sums only to nonzero formal sums but it is not acceptable. (The substitution by the unintegrated case $\mathfrak{c}$ is the identity for this particular $\mathfrak{c}$.)

An idea to test whether π_σ is acceptable would be to test whether (aside from preserving vanishing sums)

$$\texttt{SumsN0}(\mathfrak{c})\ /.\ \pi_\sigma\ /.\ \mathfrak{c} \subset \texttt{SumsN0}(\mathfrak{c})\,.$$

This would indeed guarantee that π_σ is acceptable but this condition is too restrictive.

Example B.31. The case $l[c_1, -c_1, c_3, -c_3]$ has the acceptable permutation $\sigma = (2, 1, 4, 3)$. The vanishing sums are $\{c_1 + c_2, c_3 + c_4\}$, which are preserved by π_σ:

$$\{c_1 + c_2, c_3 + c_4\} /. \pi_\sigma /. \mathfrak{c} = \{c_2 + c_1, c_4 + c_3\} /. \mathfrak{c} = \{-c_1 + c_1, -c_3 + c_3\} = \{0\}.$$

However, the nonvanishing sums are $\texttt{SumsN0}(\mathfrak{c}) = \{c_1 + c_2 + c_3, c_2 + c_3\}$ and we have

$$\texttt{SumsN0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} = \{c_2 + c_1 + c_4, c_1 + c_4\} /. \mathfrak{c} = \{-c_3, c_1 - c_3\} \not\subset \texttt{SumsN0}(\mathfrak{c})$$

(even if we ignore the trivial sum $-c_3$). If we are given nonvanishing sums $\texttt{SumsN0}(\mathfrak{c})$ then we know that the sums in $\texttt{SumsN0}(\mathfrak{c}) /. \mathfrak{c}$ are also nonvanishing. Hence, we demand that

$$\texttt{SumsN0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} \subset \texttt{SumsN0}(\mathfrak{c}) /. \mathfrak{c}.$$

The right hand side is given by $\{c_3, -c_1 + c_3\}$ and thus this condition is still not satisfied in this example. But, if $-c_1 + c_3$ is nonvanishing then $-(-c_1 + c_3)$ is also nonvanishing. We only need

$$\texttt{SumsN0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} \subset \pm\texttt{SumsN0}(\mathfrak{c}) /. \mathfrak{c}$$

and this is indeed the case for $\sigma = (2, 1, 4, 3)$.

As explained in the preceding example a permutation σ is acceptable for an (unintegrated) case if the following two conditions hold

(1) $\texttt{Sums0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} \subset \{0\}$ and

(2) $\texttt{SumsN0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} \subset \pm\texttt{SumsN0}(\mathfrak{c}) /. \mathfrak{c}$.

It follows from the discussion above that any permutation that satisfies those two conditions is acceptable. We could relax the second condition to

$$\texttt{SumsN0}(\mathfrak{c}) /. \pi_\sigma /. \mathfrak{c} \subset (\mathbb{Z}\backslash\{0\})\texttt{SumsN0}(\mathfrak{c}) /. \mathfrak{c}$$

but this does not increase the number of permutations shown to be acceptable—at least up to and including wave invariant 8. Since those wave invariants cannot be computed with present day computers using the approach presented here anyway, we may use the simpler test.

Also, we will not prove the converse, every acceptable permutation must satisfy the two conditions above, as we do not need it: We are only aiming to simplify the wave invariants and for this we need sufficiently many but not necessarily all acceptable permutations.

B.5 Maximal Q-order Term

In this section we will compute and simplify the τ- and x-integrals of the single summand with the maximal Q-order k in the k-th wave invariant $\mathsf{WI}_{k,d}(a, Q)$. We have already shown in Lemma 4.41 that in the wave invariants there is no x-dependence outside the potentials and by Lemma B.4 the order of potentials in $H(i, j, k)$ and thus $\mathsf{WI}_{k,d}(a, Q)$ is at most k.

Lemma B.32. The only summand of the partial wave invariant $\mathsf{WI}_{k,l}(Q)$ with the maximal Q-order k is of the form

$$\langle \Big(\frac{\mathrm{i}}{2}|l|\Big)^k \tau_2 \cdots \tau_k^{k-1} \prod_{i=1}^{k} Q(x + l\tau_i \cdots \tau_k), E_{-Fl}(x) \rangle \,.$$

Proof. The proof works analogously to the proofs of Lemma B.3 and 4.41 but here we only need to consider the Q-part of the wave operator and it only needs to be applied to the part with the maximal Q-order in a_i, adding a single potential for each step $a_i \to a_{i+1}$. The substitution of arguments "$\to_i$" and the single coefficient t in $a_i = \frac{\mathrm{i}}{2} t A_i$ yield the increasing τ-exponent and the factor $(\frac{\mathrm{i}}{2}|l|)^k$. □

Example B.33. We can evaluate the τ-integrals in the terms with maximal Q-order using the algorithm given in this appendix. Together with the x-integration, which implies $\Sigma\, c + Fl = 0$, the highest Q-order terms evaluate to:

$$\begin{aligned}
&\frac{\mathrm{i}}{2}|l| Q_{-Fl} && \text{for } k = 1\\
&\Big(\frac{\mathrm{i}}{2}|l|\Big)^2 \sum_{c \in l[0,0]}^{Q} \frac{1}{2} && \text{for } k = 2\\
&\Big(\frac{\mathrm{i}}{2}|l|\Big)^3 \sum_{c \in l[0,0,0]}^{Q} \frac{1}{6} && \text{for } k = 3
\end{aligned}$$

We might be tempted to believe that the summand equals

$$\Big(\frac{\mathrm{i}}{2}|l|\Big)^k \sum_{c \in l[0,\dots,0]}^{Q} \frac{1}{k!} \qquad \text{for all } k \in \mathbb{N},$$

and, indeed, this term must always appear. However, for $k \geq 4$ the τ-integrals give additional terms, as well. The term with maximal Q-order for $k = 4$ is

$$\Big(\frac{\mathrm{i}}{2}|l|\Big)^4 \Big[\sum_{c \in l[0,0,0,0]}^{Q} \frac{1}{4!} + \sum_{\substack{c \in l[c_1,-c_1,c_1,-c_1] \\ \cup l[c_1,-c_1,c_3,-c_3]}}^{Q} \frac{1}{2\tilde{c}_1(l)\tilde{c}_3(l)} \Big].$$

For $k = 5$ we have

$$\begin{aligned}\Big(\frac{\mathrm{i}}{2}|l|\Big)^5\Big[&\sum_{c\in I[0,0,0,0,0]}^{Q} \frac{1}{5!} + \sum_{\substack{c\in I[0,c_2,-c_2,c_2,-c_2]\\ \cup I[0,c_2,-c_2,c_4,-c_4]}}^{Q} \frac{1}{2\tilde{c}_2(l)\tilde{c}_4(l)} \\ &+ \sum_{c\in I[c_1,-c_1,c_3,c_4,-c_3-c_4]}^{Q} \frac{(\tilde{c}_1(l)+\tilde{c}_3(l))\tilde{c}_5(l)-\tilde{c}_1(l)\tilde{c}_3(l)}{\tilde{c}_1(l)^2\tilde{c}_3(l)^2\tilde{c}_5(l)^2} \\ &+ \sum_{c\in I[c_1,c_2,-c_2,c_2,-c_1-c_2]}^{Q} 2\frac{\tilde{c}_1(l)^2+\tilde{c}_1(l))\tilde{c}_2(l)+\tilde{c}_2(l)^2}{\tilde{c}_1(l)^2\tilde{c}_2(l)^2\tilde{c}_5(l)^2} \\ &+ \quad 8 \text{ other similar sums} \quad \Big].\end{aligned}$$

It will turn out, though, that those additional terms cancel and that the initial conjecture is indeed true.

Lemma B.34. For $k \in \mathbb{N}$ let $\mathcal{S}_k$ denote the permutations of $\{1,\dots,k\}$ and for $h \in \mathbb{N}_0^k$ with $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ let

$$B(h) := \prod_{i=1}^{k} \frac{1}{i+h_1+\cdots+h_i}.$$

Then

$$S(h) := \sum_{\pi\in\mathcal{S}_k} B(h_\pi) = \frac{1}{(1+h_1)\cdots(1+h_k)}.$$

Proof. The claim is trivial for $k = 1$. Consider $k+1$ and $h \in \mathbb{N}_0^{k+1}$. We have by induction

$$\begin{aligned}S(h) &= \sum_{\pi\in\mathcal{S}_{k+1}} B(h_\pi) = \sum_{\pi\in\mathcal{S}_{k+1}} \prod_{i=1}^{k+1} \frac{1}{i+h_{\pi 1}+\cdots+h_{\pi i}} \\ &= \sum_{\pi\in\mathcal{S}_k} \prod_{i=1}^{k} \frac{1}{i+h_{\pi 1}+\cdots+h_{\pi i}} \cdot \frac{1}{k+1+h_{\pi 1}+\cdots+h_{\pi(k+1)}} \\ &= \sum_{\pi_{k+1}=1}^{k+1} \sum_{\pi\in\mathcal{S}_k} B((h_1,\dots,\hat{h_{\pi_{k+1}}},\dots,h_{k+1})_\pi) \frac{1}{k+1+h_1+\cdots+h_{k+1}} \\ &= \sum_{\pi_{k+1}=1}^{k+1} S(h_1,\dots,\hat{h_{\pi_{k+1}}},\dots,h_{k+1}) \frac{1}{k+1+h_1+\cdots+h_{k+1}} \\ &= \sum_{\pi_{k+1}=1}^{k+1} \frac{1+h_{\pi_{k+1}}}{(1+h_1)\cdots(1+h_{k+1})} \cdot \frac{1}{k+1+h_1+\cdots+h_{k+1}} \\ &= \frac{1}{(1+h_1)\cdots(1+h_{k+1})}.\end{aligned}$$

□

This Lemma B.34 can now be applied to the symmetrized sums over certain τ-integrals of exponential functions appearing in the Fourier series expansion of the highest Q-order term of the wave invariants.

Lemma B.35. For $k \in \mathbb{N}$ chose $(c_1, \cdots, c_k) \in (2\pi i\mathbb{Z})^k$ such that at least one of the c_i is not zero. Then

$$\sum_{\pi\in\mathcal{S}_k} \tau^e e^{c_{\pi 1}\tau_1 \cdots \tau_k} \cdots e^{c_{\pi k}\tau_k} \overset{\tau}{=} 0 \qquad \text{with } e = (0, 1, \ldots, k-1).$$

Proof. With the notation $c_\pi^h := c_{\pi 1}^{h_1} \cdots c_{\pi k}^{h_k}$ we can expand the exponentials and a rearranging of indices yields the following:

$$\begin{aligned} E(c) := \sum_{\pi\in\mathcal{S}_k} \tau^e e^{c_{\pi 1}\tau_1 \cdots \tau_k} \cdots e^{c_{\pi k}\tau_k} &= \sum_{\pi\in\mathcal{S}_k} \sum_{h\in\mathbb{N}_0^k} \frac{c_\pi^h}{h!} (\tau_1 \cdots \tau_k)^{h_1} \cdots \tau_k^{h_k} \cdot \tau^e \\ &= \sum_{\pi\in\mathcal{S}_k} \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{h!} (\tau_1 \cdots \tau_k)^{h_{\pi 1}} \cdots \tau_k^{h_{\pi k}} \cdot \tau^e \end{aligned}$$

We can compute the τ-integrals in each summand and apply Lemma B.34.

$$\begin{aligned} E(c) &= \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{h!} \sum_{\pi\in\mathcal{S}_k} \tau_1^{h_{\pi 1}} \cdot \tau_2^{h_{\pi 1}+h_{\pi 2}+1} \cdots \tau_k^{h_{\pi 1}+\cdots+h_{\pi k}+k-1} \\ &= \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{h!} \sum_{\pi\in\mathcal{S}_k} \frac{1}{1+h_{\pi 1}} \cdot \frac{1}{2+h_{\pi 1}+h_{\pi 2}} \cdots \frac{1}{k+h_{\pi 1}+\cdots+h_{\pi k}} \\ &= \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{h!} S(h) = \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{h!} \frac{1}{(1+h_1)\cdots(1+h_k)} = \sum_{h\in\mathbb{N}_0^k} \frac{c^h}{(1+h)!} \end{aligned}$$

If we assume for simplicity that $c_k \neq 0$ then

$$E(c) = \sum_{h\in\mathbb{N}_0^{k-1}} \frac{c^h}{(1+h)!} \cdot \frac{1}{c_k} \sum_{H=0}^{\infty} \frac{c_k^{H+1}}{(1+H)!}$$

and

$$\sum_{H=0}^{\infty} \frac{c^{H+1}}{(1+H)!} = \sum_{H=0}^{\infty} \frac{c^H}{(H)!} - 1 = e^{c_k} - 1 = 0\,,$$

because $c_k \in 2\pi i\mathbb{Z}$. The claim follows. □

With this Lemma we can compute the highest Q-order terms of the partial wave invariants.

Lemma B.36. For every $k \in \mathbb{N}$ and every smooth, periodic potential Q we have that the highest Q-order term in the k-th partial wave invariant $\mathsf{WI}_{k,l}(Q)$ is equal to

$$\left(\frac{\mathrm{i}}{2}|l|\right)^k \langle \tau_2 \cdots \tau_k^{k-1} \prod_{i=1}^{k} Q(\,.\, + l\tau_i \cdots \tau_k), E_{-Fl} \rangle = \left(\frac{\mathrm{i}}{2}|l|\right)^k \sum_{c \in l[0,\ldots,0]}^{Q} \frac{1}{k!}\,.$$

Proof. Using the Fourier expansion of Q and $e = (0, \ldots, k-1)$ gives

$$I_k \coloneqq \tau^e \prod_{i=1}^{k} Q(\,.\, + l\tau_i \cdots \tau_k) = \sum_{c \in \mathcal{L}'^k} Q_c E_c(x) \cdot \tau^e E_{c_1}(l\tau_1 \cdots \tau_k) \cdots E_{c_k}(l\tau_k)$$

and by Lemma B.35 those summands of I_k that are equal up to permutation cancel unless all $c_i(l) = 0$. Thus,

$$I_k \overset{\tau}{=} \sum_{c_i(l)=0} Q_c E_c(x) \cdot \tau^e \overset{\tau}{=} \sum_{c_i(l)=0} Q_c E_c(x) \cdot \frac{1}{k!} \quad \text{and} \quad \langle I_k, E_{-Fl} \rangle = \sum_{c \in l[0,\ldots,0]}^{Q} \frac{1}{k!}\,. \qquad \square$$

Appendix C

Mathematica Code: Heat Invariants

This Appendix contains the MATHEMATICA *notebook* used to compute unintegrated higher heat invariants. The notebook requires the computer algebra system MATHEMATICA [MMA15]. An introduction to MATHEMATICA can be found in [MMA08].

The notebook is avialable in digital form [Ber18].

In this notebook some more technical facts relating to integration by parts are used, which shall be given before the implementation of the MATHEMATICA notebook.

C.1 Integration by Parts

While we cannot perform the x-integration of the heat invariants outright without a more specific choice of Q, we can use integration by parts to simplify the results of the computation of the heat invariants.

Lemma C.1 (Integration by Parts).
If $f, g\colon \mathbb{R}^n \to \mathbb{C}$ are two $\mathcal{L}$-periodic smooth function, $\mathcal{F}$ a unit cell of $\mathcal{L}$ and $v \in \mathbb{R}^n\backslash\{0\}$, then

$$\int_{\mathcal{F}} \partial_v f(x) \cdot g(x)\,\mathrm{d}x = -\int_{\mathcal{F}} f(x) \cdot \partial_v g(x)\,\mathrm{d}x\,.$$

Proof. For the case $\mathcal{F} = [0,1]^n$ the claim follows from the conventional integration by parts (with respect to each of the components $\partial_v = v^i\partial_i$). For the general case we use an isomorphism $A\colon \mathbb{R}^n \to \mathbb{R}^n$ with $A[0,1]^n = \mathcal{F}$ and integration by substitution:

$$\int_{\mathcal{F}} (\partial_v f)(x) \cdot g(x)\,\mathrm{d}x = \int_{[0,1]^n} (\partial_v f)(Ay) g(Ay) |\det A|\,\mathrm{d}y\,.$$

If f' denotes the Jacobian of f then

$$(f \circ A)' = f' \circ A \cdot A' = f' \circ A \cdot A \qquad \text{and} \qquad \partial_v f = f' v\,.$$

Thus, the integral is equal to

$$\begin{aligned}\int_{[0,1]^n} f'(Ay)v \cdot g(Ay)|\det A|\,\mathrm{d}y &= \int_{[0,1]^n} f'(Ay)AA^{-1}v \cdot g(Ay)|\det A|\,\mathrm{d}y \\ &= \int_{[0,1]^n} \partial_{A^{-1}v}(f \circ A)(y) \cdot g(Ay)|\det A|\,\mathrm{d}y\,.\end{aligned}$$

This is the $\mathcal{F} = [0,1]^n$-case and the partial derivative can be moved onto g. Substituting the resulting integral back to $\mathcal{F}$ gives the claim. □

We write $f_i \coloneqq \partial_i f$. Recall that $f \approx g$ if $\int_{\mathcal{F}} f(x)\,\mathrm{d}x = \int_{\mathcal{F}} g(x)\,\mathrm{d}x$. The partial integration can be written as $f_i g \approx -f g_i$, for example.

Let Q be an $\mathcal{L}$-periodic smooth potential $Q\colon \mathbb{R}^n \to \mathbb{R}$ and $k \in \mathbb{N}$. Also, in the following Lemmata the Einstein convention is used in the sense that all indices i, j or i_s are summed over 1 to n.

Lemma C.2 (IBP 1 and IBP 2).

$$Q_{i_1,\dots,i_k} \approx 0 \qquad \text{and} \qquad (\Delta^k Q_{i_1,\dots,i_h})^2 \approx (-1)^h Q \cdot \Delta^{2k+h} Q$$

Proof. The first equation follows from $Q_{i_1,\dots,i_k} \cdot 1 \approx -Q_{i_2,\dots,i_k}\partial_{i_1} 1 = 0$. The second follows analogously with $Q_{i,i} = \Delta Q$. □

Further, we abbreviate $Q_{i_1,\dots,i_h} = Q_I$ with $I = \{i_1, \dots, i_h\}$.

Lemma C.3 (IBP 3).

$$\Delta^{l_1} Q \cdot \Delta^{l_1} Q_i \cdot \Delta^{l_2} Q_j \approx -\frac{1}{2}(\Delta^{l_1} Q)^2 \cdot \Delta^{l_2} Q_{i,j} \tag{C.1}$$

$$\Delta^{l_1} Q_I \cdot \Delta^{l_1} Q_{I,i} \cdot \Delta^{l_2} Q_i \approx -\frac{1}{2}(\Delta^{l_1} Q_I)^2 \cdot \Delta^{l_2+1} Q \tag{C.2}$$

$$\Delta^k Q_i \cdot \Delta^k Q_j \cdot \Delta^{k+1} Q_{i,j} \approx \frac{1}{2}(\Delta^k Q_i)^2 \cdot \Delta^{k+2} Q + \frac{1}{2}(\Delta^{k+1} Q)^3 \tag{C.3}$$

$$\Delta^{l_1} Q_I \cdot (\Delta^{l_2} Q_{J,j})^2 \approx \frac{1}{2}(\Delta^{l_2} Q_J)^2 \cdot \Delta^{l_1+1} Q_I - \Delta^{l_2} Q_J \cdot \Delta^{l_2+1} Q_J \cdot \Delta^{l_1} Q_I \tag{C.4}$$

Proof. Integration by parts gives

$$\Delta^{l_1} Q \cdot \Delta^{l_1} Q_i \cdot \Delta^{l_2} Q_j \approx -\Delta^{l_1} Q_i \cdot \Delta^{l_1} Q \cdot \Delta^{l_2} Q_j - \Delta^{l_1} Q \cdot \Delta^{l_1} Q \cdot \Delta^{l_2} Q_{i,j}\,.$$

Equation C.1 follows. Equation C.2 follows analogously with $\Delta^{l_2} Q_{i,i} = \Delta^{l_2+1} Q$.

For equation C.3 note first that we have for all smooth $\mathcal{L}$-periodic functions $f\colon \mathbb{R}^n \to \mathbb{R}$ by integration by parts with respect to the second i that

$$2f_j \cdot \Delta f_i \cdot f_{ij} \approx -2f_{ji} \cdot \Delta f_i \cdot f_j - 2f_j^2 \cdot \Delta^2 f \qquad \text{and thus}$$
$$2f_j \cdot \Delta f_i \cdot f_{ij} \approx -f_i^2 \cdot \Delta^2 f\,.$$

It follows that

$$\begin{aligned}(\Delta f)^3 = (\Delta f)^2 \cdot f_{ii} &\approx -2\Delta f \cdot \Delta f_i \cdot f_i = -2f_{jj} \cdot \Delta f_i \cdot f_i \\ &\approx 2f_j \cdot \Delta f_{ij} \cdot f_i + 2f_j \cdot \Delta f_i \cdot f_{ij} \approx 2f_j \cdot \Delta f_{ij} \cdot f_i - f_i^2 \cdot \Delta^2 f\,.\end{aligned}$$

We obtain equation C.3 by setting $f \coloneqq \Delta^k Q$.

Finally, setting $f \coloneqq \Delta^{l_1} Q_I$ and $g \coloneqq \Delta^{l_2} Q_J$ in

$$g^2 \cdot \Delta f \approx \Delta(g^2) \cdot f = 2g \cdot \Delta g \cdot f + 2f \cdot g_j^2$$

yields equation C.4. □

Lemma C.4 (IBP4).

$$\Delta^{l_1} Q \cdot \Delta^{l_2} Q_I \cdot (\Delta^{l_1} Q_i)^2 \approx \frac{1}{6}(\Delta^{l_1} Q)^3 \cdot \Delta^{l_2+1} Q_I - \frac{1}{2}(\Delta^{l_1} Q)^2 \cdot \Delta^{l_2} Q_I \cdot \Delta^{l_1+1} Q$$

Proof. We have for all smooth $\mathcal{L}$-periodic functions $f, g\colon \mathbb{R}^n \to \mathbb{R}$ that

$$g^3 \cdot \Delta f \approx \Delta(g^3) \cdot f = 6g \cdot g_i g_i \cdot f + 3g^2 \cdot \Delta g \cdot f \qquad \text{and thus}$$
$$g \cdot f \cdot g_i g_i \approx \frac{1}{6} g^3 \cdot \Delta f - \frac{1}{2} g^2 \cdot f \cdot \Delta g\,.$$

The claim follows with $g \coloneqq \Delta^{l_1} Q$ and $f \coloneqq \Delta^{l_2} Q_I$. □

Lemma C.5 (IBP other).

$$(\Delta^{l_1} Q)^k \cdot \Delta^{l_1} Q_i \cdot \Delta^{l_2} Q_i \approx -\frac{(\Delta^{l_1} Q)^{k+1} \cdot \Delta^{l_2+1} Q}{k+1}$$
$$(\Delta^h Q)^k \cdot (\Delta^h Q_i)^2 \approx -\frac{(\Delta^h Q)^{k+1} \cdot \Delta^{h+1} Q}{k+1}$$

Proof. The first statement follows from

$$f^{k+1} \cdot \Delta g \approx -(f^{k+1})_i \cdot g_i = -(k+1) f^k \cdot f_i \cdot g_i$$

with $f \coloneqq \Delta^{l_1} Q$ and $g \coloneqq \Delta^{l_2} Q$. The second statement is a special case of the first statement with $h \coloneqq l_1 = l_2$. □

Heat Invariants

by Tillmann Berg

In this *Mathematica* notebook the first 14 heat invariants of Schrödinger operators on flat tori will be given. The calculation uses the procedure described in Chapter 3.

The results, the code and the explanations thereof can be accessed by double-clicking on the cell-brackets on the right hand side of this notebook. Pressing `Shift-Enter` within an `Input Cell` will execute this cell. Upon executing this notebook *Mathematica* will ask whether it is allowed to execute the so-called `Initialization Cells`. Allowing *Mathematica* to do so is required as these cells contain the definitions needed to construct the following function.

`HeatInvariant[`k`]`
: returns the k-th heat invariant.

```
HeatInvariant[k_] :=
 HeatInvariant[k] = CSimplify@IntegrateXi@e[k]
```

Computing the heat invariants involves three steps: First the unintegrated invariants `e[`h`]` are computed and then the integral with respect to ξ is evaluated. This does give correct but unnecessarily long and complex heat invariants. The custom simplification function `CSimplify` shortens the invariants. The functions involved are defined and explained below.

Warning: The memory requirement for the computation of the heat invariants beyond the 12th grows rapidly with the index of the invariants. Running those computations on a computer with insufficient memory may cause *Mathematica* and possibly other programs to freeze or crash and may cause a loss of data.

This *Mathematica* notebook was developed for *Mathematica* 10.3.1.0.

0.1 Technicalities

Before diving into the calculation of the heat invariants there are two minor technicalities to take care of. Firstly, we do not want *Mathematica* to abort the calculation of heat invariants because the number of nested functions exceeds the `$RecursionLimit`. This limit can be removed by setting it to `Infinity`.

Secondly, the following functions is the frequently used negation of `FreeQ`.

`ContainsQ[`*exp*`,`*pat*`]`
yields `True` if the pattern *pat* is contained in the expression *exp*, and yields `False` otherwise.

```
$RecursionLimit = Infinity;
ContainsQ[exp_, pat_] := Not@FreeQ[exp, pat]
```

For example,

```
ContainsQ[Q[x], x]
```

```
True
```

1 Approximate Resolvent

To define and compute the symbols `r[`*h*`]` of the approximate resolvent we need to define three things: Curvature traces, potentials and derivatives thereof. Also, the definition of the symbols of the approximate resolvent and their integration with respect to λ is given here. The integration with respect to ξ is more involved and follows in the next section.

1.1 Curvature Traces

`Ft[`*i*`,`*X*`,`*Y*`]` and `Ft[`*i*`]`
do not evaluate. They represent the *i*th curvature trace with vectors *X* and *Y*, or without vectors.

More precisely, `Ft` represents $\tilde{F}$ and thus a factor $2\pi i$ is included within this name. There are some simplifications that can be applied to curvature traces. By Lemma 3.9 the curvature traces of odd order are antisymmetric.

```
Ft[_?OddQ, X_, X_] := 0
```

Further, traces over curvature traces can be merged. Here such traces appear as sums over standard base vectors e_i. The sums will not be made explicit in the formulae as the Einstein summation convention is assumed.

`ei[k]`
does not evaluate, represents the standard basis vector e_{i_k}.

Note that `ei[k]` does *not* represent the kth basis vector but the i_kth basis vector and that it is assumed that all indices that appear in any formula are summed over from 1 to the dimension n of the torus. It is obvious from the definition of the symbols `r[h]` that each index k of basis vectors `ei[k]` has quadratic order, if it is present, and, therefore, is a trace. The following rules hold.

```
FtRules = {
    Ft[i_, ei[k_], ei[k_]] → Ft[i],
    Ft[i1_, X_, ei[k_]] * Ft[i2_, ei[k_], Y_] →
     Ft[i1 + i2, X, Y],
    Ft[i1_, X_, ei[k_]] * Ft[i2_, Y_, ei[k_]] →
     Ft[i1 + i2, X, Y] * (-1)^i2,
    Ft[i1_, ei[k_], x] * Ft[i2_, ei[k_], Y_] →
     Ft[i1 + i2, Y, x] * (-1)^i2,
    Ft[i1_, ei[k_], X_] * Ft[i2_, ei[k_], Y_] →
     Ft[i1 + i2, X, Y] * (-1)^i1,
    Ft[i_, X_, _ei]^2 | Ft[i_, _ei, X_]^2 → Ft[2 i, X, X] * (-1)^i
   };
```

The parity of the curvature traces is, of course, not known to *Mathematica.* Hence, formally distinct but mathematically equal expressions have to be encoded explicitly and seperately.

Example

```
(i r0^3 Ft[1, xi, ei[-3]] Ft[1, ei[-3], x]) /. FtRules
```

```
i r0^3 Ft[2, xi, x]
```

1.2 Derivatives

`dx[k, exp]` and `dx[xi, exp]`
give the derivative of *exp* with respect to `x` in the direction of `ei[k]` or `xi`.

A derivative with respect to k is *not* a derivative in the direction of the kth standard basis vector but a derivative with respect to e_{i_k}. Those indices are implicitly summed over by the Einstein convention. This derivative contains no factors *(-i)* as those will be included explicitly in the definition of the symbols `r[k]` below. The first transformation rules define the linearity and the Leibniz rule.

```
dx[X_, exp_Plus] := dx[X, #] & /@ exp
dx[X_, exp1_ * exp2_] := dx[X, exp1] * exp2 + exp1 * dx[X, exp2]
dx[X_, exp_^h_] := h * exp^(h - 1) dx[X, exp]
dx[_, exp_ /; FreeQ[exp, x]] := 0
```

The curvature traces `Ft` are bilinear and thus the Leibniz rule applies. We can use the parity of `Ft` to simplify and partially sort the result of a derivation. All `x` remaining after the derivation are in the rightmost position, which reduces ambiguity of the involved expressions and thus decreases the memory requirements of the computation.

```
dx[k_, Ft[i_, x, x]] := 2 Ft[i, ei[k], x]
dx[xi, Ft[i_, x, x]] := 2 Ft[i, xi, x]
```

If i is odd `Ft[i,x,x]` vanishes. If i is even the symmetry of `Ft[i,.,.]` gives the right hand side. Further, if an argument of `Ft` is not `x` then it must be free of `x`. There is no need to test whether an argument contains `x`.

```
dx[k_, Ft[i_, x, exp_]] := Ft[i, ei[k], exp]
dx[k_, Ft[i_, exp_, x]] := Ft[i, exp, ei[k]]
dx[xi, Ft[i_, x, exp_]] := (-1)^i Ft[i, exp, xi]
dx[xi, Ft[i_, exp_, x]] := Ft[i, exp, xi]
```

1.3 Potentials

Because the Laplacians and other derivatives of the potential `Q` cannot be computed without a specific choice of potential those derivatives will merely be collected within the potential.

`Q[x, lap, der]`
does not evaluate. Represents the potential `Q` at the point `x` with *lap* Laplacians applied and after being derived with respect to the vectors in the `List` *der*.

If the function `Q[x, lap, der]` is differentiated with respect to `ei[k]` or `xi` then this vector is added to the `List` of derivatives *der*. If, however, the vector `ei[k]` is already contained in the list of derivatives then a second derivation in the direction of `ei[k]` gives, together with the Einstein convention, a Laplacian. Thus, this vector is instead removed from the list of derivatives and the count of Laplacians *lap* is increased by one.

```
dx[k_, Q[x, lap_, der_]] := Q[x, lap, Append[der, ei[k]]]
dx[xi, Q[x, lap_, der_]] := Q[x, lap, Append[der, xi]]
dx[k_, Q[x, lap_, der_]] /; ContainsQ[der, ei[k]] :=
 Q[x, lap + 1, DeleteCases[der, ei[k]]]
```

Examples

```
dx[1, Q[x, 0, {}]]
```

```
Q[x, 0, {ei[1]}]
```

```
dx[xi, %]
```

```
Q[x, 0, {ei[1], xi}]
```

```
dx[1, %]
```

```
Q[x, 1, {xi}]
```

1.4 Symbols

`r[h]`
returns the *h*th symbol of the approximate resolvent. The recursive formula is given by Lemma 3.10.

To avoid variable conflicts the indices within the derivatives `dx` are chosen to be negative, while those used for multitraces later will have positive indices. Using `Expand` in every recursion step is not necessary but is more time and, more importantly, memory efficient. The same holds for the application of the simplifying `FtRules`. Note that in the computation of the nth heat invariant the following λ-integration needs the last symbol `r[h]` in expanded form.

Memoization is used in the recursive definition. This gives much faster computations but changes to the definition of those `r[h]` that have already been computed will have no effect unless `Clear` is used or the Kernel restarted.

```
r[-2] = 0;
r[-1] = 0;
r[0] = r0;

r[h_] :=
 r[h] =
  Expand[-r0 (Ft[2, x, x] / 4 + Q[x, 0, {}]) r[h - 2] +
       I Ft[1, xi, x] r0 r[h - 1] + I r0 2 dx[xi, r[h - 1]]] +
    Expand[r0 Ft[1, ei[-h], x]  dx[-h, r[h - 2]] +
      r0 dx[-h, dx[-h, r[h - 2]]] ] /. FtRules
```

Examples

```
r[1]
```

```
i r0^2 Ft[1, xi, x]
```

```
r[2]
```

$$-\mathrm{r0}^3\,\mathrm{Ft}[1,\mathrm{xi},\mathrm{x}]^2-\frac{1}{4}\mathrm{r0}^2\,\mathrm{Ft}[2,\mathrm{x},\mathrm{x}]-\mathrm{r0}^2\,\mathrm{Q}[\mathrm{x},0,\{\}]$$

1.5 λ-Integration

`e[h]`
: is the integral of `r[h]` with respect to $e^{-\lambda}\,d\lambda$ but does still depend on ξ, see definition 3.12.

The complex variable λ in the symbols `r[h]` appears only within `r0`. By section 3.2.1 the λ-integration of r_0^k gives $1/(k-1)!$ and the following rule implement the λ-integration.

Of course, this is only correct if the symbol `r[h]` is in expanded form, which it is. Also, the λ-integration gives a factor Exp(-|ξ|^2), but this factor is contained in every summand of `e[h]` exactly once and can therefore be ommitted in the following expressions. We do the same for normalisation constants.

```
e[h_] := r[h] /. r0^k_. → 1 / (k - 1)! /.
  Q[x, lap_, der_] → Q[lap, der]
```

For technical reasons it is beneficial to remove the `x` from the potentials at this point. It was only needed to calculate derivatives with respect to `x`.

Examples

```
e[0]
```

```
1
```

```
e[1]
```

```
i Ft[1, xi, x]
```

```
e[2]
```

$$-\frac{1}{2}\,\text{Ft}[1,\text{xi},\text{x}]^2-\frac{1}{4}\,\text{Ft}[2,\text{x},\text{x}]-\text{Q}[0,\{\}]$$

2 ξ-Integration

So far we have defined the local unintegrated invariants `e[h]`, which depend on `x` and `xi`. To compute the heat invariants from this data we need to integrate `e[h]` with respect to `xi`.

`IntegrateXi[exp]`
gives the ξ-integral of *exp* $\text{Exp}\left[-|\xi|^2\right]$ up to a factor $\pi^{n/2}$.

By Theorem 3.20 the integrals over `xi` are given by multitraces of multilinear maps. But first we need to transform the polynomials in `xi` that appear as summands within `e[h]` into multilinear maps in `xi`. `IntegrateXi` returns its result in expanded form.

2.1 Generating multilinear maps

The reason why we cannot simply evaluate multitraces from the summands themselves

is that these summands need not be linear in some `xi`, because of the existence of powers. Thus, the summands will be transformed into “custom” products with `CTimes` as a new `Head` instead of `Power` and `Times` (up to factors that are free of `xi`).

`CTimes[`*exp1*`,`*exp2*`,...]`
: does not evaluate and represents the product of its arguments. Equal arguments are *not* simplified to powers.

`ToCTimes[`*exp*`]`
: transforms *exp* into an expression that is linear in each `xi`. Assumes that *exp* is as single summand.

So, if *exp* happens to be an expression b^h with `Power` as `Head` and such that the base b contains a `xi` then `ToCTimes[`*exp*`]` returns a custom product with h equal factors b.

```
ToCTimes[b_^h_. /; ContainsQ[exp, xi]] := CTimes @@ Table[exp, h]
```

If *exp* happens to be a product then all powers within this product are replaced by such custom products. Note that because the pattern `_^h_.` also includes exponentiations with exponent *1*, which are expressions that do not have `Power` as `Head`, such subexpressions do not have to be considered separately. Since this transformation can lead to products with `CTimes` appearing as the `Head` of several factors we let the products of `CTimes` merge via the use of `UpValues`.

```
ToCTimes[exp_Times] :=
 Replace[exp, (b_ /; ContainsQ[b, xi])^h_. :>
   CTimes @@ Table[b, h] , {1}]
CTimes /: exp1_CTimes * exp2_CTimes := Join[exp1, exp2]
```

Finally, if an expression is free of `xi` then the expression itself is returned. If it is any other expression, i.e. not a product, power and not free of `xi`, then a custom product with the expression as the single factor is returned.

```
ToCTimes[exp_ /; FreeQ[exp, xi]] := exp
ToCTimes[exp_] := CTimes@exp
```

For example,

```
ToCTimes[3 Ft[xi, xi]^2]
```

```
3 CTimes[Ft[xi, xi], Ft[xi, xi]]
```

2.2 Multitrace

We have defined suitable multilinear monomials using `CTimes` and can now compute their multitraces.

`MTr[exp]`
: yields the multitrace of *exp* with respect to the variable `xi`. The expression *exp* must contain either no `CTimes` or a `CTimes` with an even number of `xi`'s.

A single trace is represented by two basis vectors `ei[k]`, where the Einstein summation convention is assumed.

Pairings

Let us call a subset of a set with cardinality 2 a *pair* and a partition of the set into pairs a *pairing*. To form the multitrace of a multilinear monomial we have to group the `xi` into pairs, replace those by `ei[k]` and sum those monomials over all pairings.

`Pairings[k]`
: returns the set of all pairings of the set *{1,...,k}*.

Of course, *k* must be even.

```
Pairings[k_] := Pairings[k] = PairingsRec@Range@k
```

`PairingsRec[list]`
: is a recursive function returning the set of all pairings of *list*.

If *list* has only two elements there is only one pairing with only one pair. If *list* has more than two elements recursion is used.

```
PairingsRec[{p1_, p2_}] := {{{p1, p2}}}
PairingsRec[list_] :=
 Join @@
  (PairAndPairings[#, PairingsRec[Complement[list, #]]] & /@
    FirstPairs[list])
```

Here,

`FirstPairs[list]`
returns a list of all pairs consisting of the first element of *list* and all other elements of *list*.

After having constructed this list of pairs with the first element of *list* we use recursion to compute the pairings of the remaining elements. Then, the pairs containing the first element are added to each pairing obtained through recursion.

`PairAndPairings[pair, pairings]`
adds *pair* to every pairing within *pairings*.

```
FirstPairs[list_] := ({First@list, #}) & /@ Drop[list, 1]
PairAndPairings[pair_, pairings_] :=
 Prepend[#, pair] & /@ pairings
```

For example,

```
FirstPairs[{1, 2, 3, 4}]
```

```
{{1, 2}, {1, 3}, {1, 4}}
```

```
Pairings[4] // Column
```

```
{{1, 2}, {3, 4}}
{{1, 3}, {2, 4}}
{{1, 4}, {2, 3}}
```

Multitrace

After having constructed the pairings we can define the multitrace. We construct the list of all pairings of the variables `xi` appearing within an expression with head `CTimes`. Then we apply a transformation given by each pairing to the expression and finally we sum over all pairings.

```
MTr[ct_CTimes] :=
 Plus @@
  (Times @@ PTr[ct, #] & /@ (Pairings@Count[ct, xi, Infinity]))
```

Here,

`PTr[ct, pairing]`
replaces the `xi` within the expression *ct* by `ei[k]` according to the *pairing*.

`Position[ct, xi]` gives the list of all positions of `xi` within the expression *ct*.

```
PTr[ct_, pairing_] :=
 ReplacePart[ct, PTrRules[Position[ct, xi], pairing]]
```

`PTrRules[positions, pairing]`
gives the rules that replace the `xi` at the *positions* with `ei[k]`, where the *positions* receive the same index according to the *pairing*.

```
PTrRules[positions_, pairing_] :=
 Rule[positions[[pairing[[#, 1]]]] |
     positions[[pairing[[#, 2]]]], ei[#]] & /@
  Range@Length@pairing
```

The `ei` are given positive indices by the `PTrRules`. Because negative indices were used in the `x`-derivatives `dx` there are no index collisions. We have for example that

```
MTr[CTimes[f[xi, xi], g[xi, xi]]]
```

```
f[ei[1], ei[2]] g[ei[1], ei[2]] +
 f[ei[1], ei[2]] g[ei[2], ei[1]] +
 f[ei[1], ei[1]] g[ei[2], ei[2]]
```

2.3 ξ-Integration

Now we have all the prerequisites to define `IntegrateXi[exp]`. Firstly, the integration is linear. If `IntegrateXi` is not applied to a sum we first convert all monomials into maps multilinear in `xi` and replace those by multitraces (times some factor). If the number of `xi` is odd the integral vanishes.

The ξ-integral also gives a factors $\pi^{n/2}$. Since this factor is present in every summand it carries no information and will be omitted. After the multiltrace is calculated we expand the result and apply the simplification rules `FtRules` to reduce the number of curvature traces `Ft` within the expression.

```
IntegrateXi[exp_Plus] := IntegrateXi /@ exp
IntegrateXi[exp_] := Expand[ToCTimes[exp] /. {
       ct_CTimes /; OddQ@Count[ct, xi, Infinity] → 0,
       ct_CTimes :> MTr@ct / 2^(Count[ct, xi, Infinity] / 2)
      }
   ] //. FtRules /. ToLaplacian
```

ToLaplacian
: is a Rule that replaces traces in the derivatives of potentials by Laplacians.

The function Tally gives a list of all elements of the list of derivatives *der* together with their multiplicity. At this point the elements of *der* are all of the form ei[*k*] and if their multiplicity is 2 then they represent a Laplacian. If their multiplicity is not 2 it must be 1 and in this case we cannot form a Laplacian. Those derivatives remain within *der*.

```
ToLaplacian =
  Q[lap_, der_] :↦ Q[lap + Count[Tally@der, eit_ /; Last@eit == 2],
    Sort@Cases[Tally@der,
      eit_ /; OddQ@Last@eit :> First@eit]];
```

Examples

```
IntegrateXi[-1/2 Ft[1, xi, x]^2]
```

$$\frac{1}{4}\,\text{Ft}[2, x, x]$$

```
1/4 Q[1, {ei[1], ei[1]}] /. ToLaplacian
```

$$\frac{1}{4}\,\text{Q}[2, \{\}]$$

```
IntegrateXi[1/2 Q[1, {xi, xi}]]
```

$$\frac{1}{4}\,\text{Q}[2, \{\}]$$

3 Simplifications

Combining the ξ-integration with the unintegrated invariants `e[h]` gives correct results for the heat invariants. However, the computed invariants so far are much longer and more complicated than they need to be.

`CSimplify[exp]`
applies some custom simplifications to *exp*.

```
CSimplify[exp_] :=
 Sortei@
  Reduceei@
   Symmetrizeei@Reduceei@IntegrationByParts@Reduceei@exp
```

The involved functions will be explained below. Using `Reduceei` twice is a bit faster, while the last `Reduceei` leads to a smaller 14th heat invariant but has no effect for lower invariants. `Symmetrizeei` gives smaller heat invariants from order 8 upwards.

3.1 Index Reduction

The indices k of `ei[k]` were chosen such that there is no index collision. Of course, this leaves considerable ambiguity. For example, the following expression contains two terms that are formally distinct but that would cancel after an appropriate renaming of indices.

```
IntegrateXi[e[4]]
```

$$-\frac{\text{Ft}[2]}{12}+\frac{1}{2}\,\text{Q}[0,\{\}]^2-\frac{1}{2}\,\text{Ft}[1,\text{ei}[-4],\text{x}]\,\text{Q}[0,\{\text{ei}[-4]\}]+\frac{1}{2}\,\text{Ft}[1,\text{ei}[1],\text{x}]\,\text{Q}[0,\{\text{ei}[1]\}]-\frac{1}{6}\,\text{Q}[1,\{\}]$$

`Reduceei[exp]`
renames the indices k of the `ei[k]` in *exp* such that the indices of each summand in *exp* range from 1 to the number of distinct indices in this summand.

Because we want the indices minimal but positive we need to apply `Reduceei` to each

summand individually. If Reduceei is applied to a summand then we use the function

RenameeiIndices[*exp*, *eiindices*]
to rename the *eiindices* within *exp* to *1* to the length of *eiindices*.

```
Reduceei[exp_Plus] := Reduceei /@ exp
Reduceei[exp_] :=
 Sortei@RenameeiIndices[exp, eiIndices@exp]

RenameeiIndices[exp_, eiindices_] :=
 exp /. Array[(ei[eiindices[[#]]] → ei[#]) &, Length@eiindices]
```

Here,

eiIndices[*exp*]
returns the list of indices *k* of the ei[*k*] within *exp* (without duplicates).

```
eiIndices[exp_] :=
 DeleteDuplicates@Cases[exp, ei[i_] → i, Infinity]
```

After reducing the ei-indices it is helpful to sort the indices within the curvature traces and the derivatives of potentials.

Sortei[*exp*]
sorts the ei-indices within *exp*.

In the case of curvature traces we have to take parity into account. Note that the only expressions with List as Head in the heat invariants must be derivative lists.

```
Sortei[exp_] :=
 exp /.
  {Ft[i_, ei[j_], ei[k_]] /; j > k → Ft[i, ei[k], ei[j]] (-1)^i,
   der_List :> Sort@der}
```

For example,

```
Reduceei[-1/2 Ft[1, ei[-4], x] Q[0, {ei[-4]}]]
```

$$-\frac{1}{2}\,\text{Ft}[1,\text{ei}[1],x]\,\text{Q}[0,\{\text{ei}[1]\}]$$

Applying `Reduceei` to the example above, `e[4]`, gives the desired cancellation.

```
Reduceei@IntegrateXi@e@4
```

$$-\frac{\text{Ft}[2]}{12}+\frac{1}{2}\,\text{Q}[0,\{\}]^2-\frac{1}{6}\,\text{Q}[1,\{\}]$$

3.2 Integration by Parts

The heat invariants are obtained from “local invariants” by an x-integration over the manifold or, in this case, a fundamental domain of the lattice. This integration can, in general, not be computed without choosing a specific potential `Q`. However, we can use integration by parts with respect to the `x`-integration to simplify the invariants.

`IntegrationByParts[`*exp*`]`
: uses integration by parts with respect to the `x`-integration in order to simplify *exp*.

This function assumes that *exp* is provided in expanded form and is applied to each summand separately. We use different transformations based on the order of the potential `Q` within each summand. The implementation of the transformations for a given `Q`-order follow below. Since the order of `Q` in a summand of the $2k$-th heat invariant is at most k, the rules have an effect only for sufficiently high heat invariants.

```
IntegrationByParts[exp_Plus] := IntegrationByParts /@ exp
IntegrationByParts[exp_] := Switch[Qorder[exp],
    -1 | 0, (* If there are x outside of Q or if there
     are no potentials then no changes can be applied. *)
        exp,
    1,
        IBP1@exp,
    2,
        IBP2@exp,
    3,
        IBP3@exp,
    4,
        IBPother@IBP4[exp],
    _, (* Qorder>4 *)
        IBPother@exp
  ] /. ToLaplacian /. Notation
```

`Qorder[exp]`
: returns the order in which the potential `Q` appears in *exp*. If there is an `x` within *exp* then *-1* is returned.

We have removed `x` from the potential `Q` at the very end of the definiton of the approximate resolvent. Therefore, any `x` that still appears in *exp* must be outside of the potential. Integration by parts is not applied in this case and to signal this we return `-1` in this case.

```
Qorder[exp_ /; ContainsQ[exp, x]] := -1
Qorder[exp_Times] := Plus @@ Qorder /@ List @@ exp
Qorder[exp_^e_] := e * Qorder[exp]
Qorder[_Q] := 1
Qorder[_] := 0
```

After using integration by parts we again use the rule `ToLaplacian` to reduce the number of traces over derivatives of potentials `Q`. Also, we can drop the count of Laplacians if it is zero and the list of other derivatives if it is empty.

`Notation`
: is a list of rules that remove trivial arguments from `Q`.

```
Notation = {Q[0, {}] → Q, Q[lap_, {}] → Q[lap],
    Q[0, der_] → Q[der], Q[0] → Q};
```

What follows now are a list of rules that are applied to summands of the corresponding Q-order. The idea is to turn traces over derivatives into Laplacians (when possible) in order to reduce the ambiguity arising from the naming of indices.

IBPk[*exp*]
: applies simplification rules based on integration by parts to *exp*, where k denotes the Q-order of *exp*.

Proofs for those transformations can be found in Lemmata C.2, C.3, C.4 and C.5.

```
IBP1[exp_] :=
 exp /. Q[lap_, der_] :> If[lap + Length@der > 0, 0, Q]

IBP2[exp_] := exp /. {
   Q[k_, der_]^2 :> (-1)^Length@der Q[2 k + Length@der] Q,
   Q[k1_, der1_] Q[k2_, der2_] :>
    (-1)^Length@der2 Q[k1 + k2, Join[der1, der2]] Q
  }

IBP3[exp_] := Expand[exp //. {
    Q[l1_, der1_] Q[l1_, der2_] Q[l2_, {ei[i_]}] /;
      Sort[Append[der1, ei[i]]] === der2 :>
     -Q[l1, der1]^2 Q[l2 + 1, {}] / 2,
    Q[l1_, {}] Q[l1_, {ei[i_]}] Q[l2_, {ei[j_]}] :>
     -1 / 2 Q[l1, {}]^2 Q[l2, Sort@{ei[i], ei[j]}],
    Q[l1_, {ei[i_]}] Q[l1_, {ei[j_]}]
       Q[l2_, {ei[i_], ei[j_]}] /; l1 + 1 == l2 :>
     Q[l1, {ei[j]}]^2 Q[l2 + 1, {}] / 2 + Q[l1 + 1, {}]^3,
    Q[l1_, der1_] Q[l2_, der2_]^2 /; Length@der2 > 0 :>
     1 / 2 Q[l2, Drop[der2, -1]]^2 Q[l1 + 1, der1] -
      Q[l2, Drop[der2, -1]] Q[l2 + 1, Drop[der2, -1]]
       Q[l1, der1]
   }]
```

```
IBP4[exp_] := Expand[exp /. {
     Q[l1_, {}] Q[l2_, der_] Q[l1_, {_ei}]^2 :>
      -1 / 2 Q[l1]^2 Q[l1 + 1] Q[l2, der] +
       1 / 6 Q[l1]^3 Q[l2 + 1, der]
    }]

IBPother[
  Q[l1_, {}]^k_. * Q[l1_, {_ei}] Q[l2_, {_ei}] * c_. /;
   FreeQ[c, _Q]] := -c Q[l1]^(k + 1) * Q[l2 + 1] / (k + 1)
IBPother[
  Q[h_, {}]^k_. * Q[h_, {_ei}]^2 * c_. /; FreeQ[c, _Q]] :=
 -c Q[h]^(k + 1) * Q[h + 1] / (k + 1)
IBPother[exp_] := exp
IBPother[exp_Plus] := IBPother /@ exp
```

3.3 Symmetrization of Indices

The indices that denote the variables that are summed over in the traces are of course arbitrary. There appear terms in the heat invariants that are zero or cancel with other terms but are formally nonvanishing. This simplification only applies to heat invariants eight and above.

Examples

The following formally nonzero term appears in the eighth heat invariant and is equal to zero, because the curvature traces `Ft` are alternating for odd indices while the derivatives of potentials are symmetric.

```
-7/12 Q Ft[1, ei[1], ei[2]] Q[{ei[1], ei[2]}]
```

```
-7/12 Q Ft[1, ei[1], ei[2]] Q[{ei[1], ei[2]}]
```

In the 12th heat invariant there are three equal but formally distinct terms, which also happens to cancel.

$$-\frac{1}{40} Q\,\text{Ft}[1, \text{ei}[1], x]\,\text{Ft}[1, \text{ei}[2], x]\,\text{Ft}[1, \text{ei}[3], x]\,Q[\{\text{ei}[3]\}]\,Q[\{\text{ei}[1], \text{ei}[2]\}] - \frac{1}{30} Q\,\text{Ft}[1, \text{ei}[1], x]\,\text{Ft}[1, \text{ei}[2], x]\,\text{Ft}[1, \text{ei}[3], x]\,Q[\{\text{ei}[2]\}]\,Q[\{\text{ei}[1], \text{ei}[3]\}] + \frac{7}{120} Q\,\text{Ft}[1, \text{ei}[1], x]\,\text{Ft}[1, \text{ei}[2], x]\,\text{Ft}[1, \text{ei}[3], x]\,Q[\{\text{ei}[1]\}]\,Q[\{\text{ei}[2], \text{ei}[3]\}];$$

Implementation

Instead of trying to somehow recognize summands that only differ by a permutation of indices the idea is to instead “symmetrize” all summands.

`Symmetrizeei[`*exp*`]`
: transforms the expression *exp* into an equal sum of expressions where the indices *k* of the traces given by `ei[`*k*`]` are permuted in every possible way.

`Symmetrizeei` is linear and if there are less than two indices then nothing can be permuted. `Symmetrizeei` generates a sum with as many summands as there are permutations. All summands are equal. Thus, each summand must be divided by the number of permutations for the sum to be equal to *exp*. Further, merely permuting the indices would not give cancellation. We also need to sort the indices according to `Sortei`.

```
Symmetrizeei[exp_Plus] := Symmetrizeei /@ exp
Symmetrizeei[exp_] := If[Length@eiIndices@exp < 2,
  (* then *)     exp,
  (* else *)     Sortei@With[
                      {eip = eiPermutations@exp},
                      (Plus @@ ((exp /. eip) / Length@eip))
   ]
 ]
```

Here,

`eiPermutations[`*exp*`]`
: returns a `List` of lists of transformation rules, where each of the latter lists corresponds to one permutation of the indices in *exp*

```
eiPermutations[exp_] := With[{ind = eiIndices[exp]},
  PermToeiRule[ind, #] & /@ Permutations[ind]
 ]
```

and

PermToeiRule[*ind*,*perm*]
uses the List of indices *ind* and a single permutation *perm* thereof to return a List of rules that substitute the ei-indices correspondingly.

Trivial rules are removed.

```
PermToeiRule[ind_, perm_] :=
 Map[ei@# &,
      Rule @@@ Replace[Transpose@{ind, perm},
    {i_, i_} → Sequence[], {1}],
  {2}]
```

For example, we have the following list of permutations.

```
eiPermutations[f[ei[1], ei[2], ei[3]]] // Column
```

```
{}
{ei[2] → ei[3], ei[3] → ei[2]}
{ei[1] → ei[2], ei[2] → ei[1]}
{ei[1] → ei[2], ei[2] → ei[3], ei[3] → ei[1]}
{ei[1] → ei[3], ei[2] → ei[1], ei[3] → ei[2]}
{ei[1] → ei[3], ei[3] → ei[1]}
```

Examples

If we now apply Symmetrizeei to the initial examples we have

```
Symmetrizeei[-7/12 Q Ft[1, ei[1], ei[2]] Q[{ei[1], ei[2]}]]
```

```
0
```

and

```
Symmetrizeei[
 -1/40 Q Ft[1, ei[1], x] Ft[1, ei[2], x] Ft[1, ei[3], x]
  Q[{ei[3]}] Q[{ei[1], ei[2]}] -
 1/30 Q Ft[1, ei[1], x] Ft[1, ei[2], x] Ft[1, ei[3], x]
  Q[{ei[2]}] Q[{ei[1], ei[3]}] +
 7/120 Q Ft[1, ei[1], x] Ft[1, ei[2], x] Ft[1, ei[3], x]
  Q[{ei[1]}] Q[{ei[2], ei[3]}]]
```

```
0
```

as desired.

4 Results

With the definitions of the previous sections we obtain the following unintegrated heat invariants. We briefly repeat the notation needed for the results.

`Q` and `Q[k]` and `Q[k,d]`
: denote the potential Q and $\Delta^k Q$ and $\Delta^k Q_d$ with derivatives d respectively.

`Ft[k,X,Y]` and `Ft[k]`
: are curvature traces defined in Definition 3.7 times the factor $(2\pi i)^k$.

`ei[k]`
: denotes the standard basis vectors e_{i_k} where the Einstein convention is understood.

```
HeatInvariant[0]
```

```
1
```

```
HeatInvariant[2]
```

```
-Q
```

HeatInvariant[4]

$$\frac{Q^2}{2} - \frac{Ft[2]}{12}$$

HeatInvariant[6]

$$-\frac{Q^3}{6} + \frac{1}{12} Q\, Ft[2] + \frac{1}{12} Q\, Q[1]$$

HeatInvariant[8]

$$\frac{Q^4}{24} - \frac{1}{24} Q^2\, Ft[2] + \frac{Ft[2]^2}{288} + \frac{Ft[4]}{360} - \frac{1}{24} Q^2\, Q[1] + \frac{1}{120} Q\, Q[2]$$

HeatInvariant[10]

$$-\frac{Q^5}{120} + \frac{1}{72} Q^3\, Ft[2] - \frac{1}{288} Q\, Ft[2]^2 - \frac{1}{360} Q\, Ft[4] + \frac{1}{72} Q^3\, Q[1] - \frac{1}{144} Q\, Ft[2]\, Q[1] - \frac{1}{360} Q\, Q[1]^2 - \frac{1}{360} Q^2\, Q[2] + \frac{Q\, Q[3]}{1680} - \frac{1}{180} Q\, Ft[2, ei[1], ei[2]]\, Q[\{ei[1], ei[2]\}]$$

HeatInvariant[12]

$$\frac{Q^6}{720} - \frac{1}{288} Q^4\, Ft[2] + \frac{1}{576} Q^2\, Ft[2]^2 - \frac{Ft[2]^3}{10\,368} + \frac{1}{720} Q^2\, Ft[4] - \frac{Ft[2]\, Ft[4]}{4320} - \frac{Ft[6]}{5670} - \frac{1}{288} Q^4\, Q[1] + \frac{1}{288} Q^2\, Ft[2]\, Q[1] - \frac{149\, Q[1]^3}{45\,360} - \frac{Q^3\, Q[2]}{2160} - \frac{Q\, Ft[2]\, Q[2]}{1440} + \frac{13\, Q\, Q[1]\, Q[2]}{30\,240} + \frac{11\, Q^2\, Q[3]}{8640} + \frac{Q\, Q[4]}{30\,240} + \frac{1}{288} Q[\{ei[1]\}]^2\, Q[\{ei[2]\}]^2 + \frac{1}{360} Q^2\, Ft[2, ei[1], ei[2]]\, Q[\{ei[1], ei[2]\}] + \frac{1}{60} Q\, Q[\{ei[1]\}]\, Q[\{ei[2]\}]\, Q[\{ei[1], ei[2]\}] + \frac{1}{180} Q^2\, Q[\{ei[1], ei[2]\}]^2 - \frac{4\, Q[\{ei[1], ei[2]\}]\, Q[\{ei[1], ei[3]\}]\, Q[\{ei[2], ei[3]\}]}{2835} - \frac{1}{840} Q\, Ft[2, ei[1], ei[2]]\, Q[1, \{ei[1], ei[2]\}] - \frac{1}{280} Q\, Q[\{ei[1], ei[2]\}]\, Q[1, \{ei[1], ei[2]\}]$$

4.1 Heat Invariant 14

Heat invariant 14 takes around 20 minutes to compute and requires 2.4 GB of memory.

HeatInvariant[14]

$$-\frac{Q^7}{5040}+\frac{Q^5\,Ft[2]}{1440}-\frac{Q^3\,Ft[2]^2}{1728}+\frac{Q\,Ft[2]^3}{10\,368}-\frac{Q^3\,Ft[4]}{2160}+\frac{Q\,Ft[2]\,Ft[4]}{4320}+$$
$$\frac{Q\,Ft[6]}{5670}+\frac{Q^5\,Q[1]}{1440}-\frac{1}{864}Q^3\,Ft[2]\,Q[1]+\frac{Q\,Ft[2]^2\,Q[1]}{3456}+\frac{Q\,Ft[4]\,Q[1]}{4320}+$$
$$\frac{Q^3\,Ft[2,ei[1],ei[2]]\,Q[1]}{1080}-\frac{1}{432}Q^3\,Q[1]^2+\frac{Q\,Ft[2]\,Q[1]^2}{4320}+\frac{Q\,Q[1]^3}{1296}+$$
$$\frac{Q^4\,Q[2]}{1440}+\frac{Q^2\,Ft[2]\,Q[2]}{4320}+\frac{Q^2\,Q[1]\,Q[2]}{1440}-\frac{Q[1]^2\,Q[2]}{5400}-\frac{Q\,Q[2]^2}{7200}-\frac{Q^3\,Q[3]}{6048}-$$
$$\frac{Q\,Ft[2]\,Q[3]}{20\,160}-\frac{559\,Q\,Q[1]\,Q[3]}{907\,200}+\frac{559\,Q^2\,Q[4]}{1\,814\,400}+\frac{Q\,Q[5]}{665\,280}-\frac{1}{144}Q^2\,Q[1]\,Q[\{ei[1]\}]^2+$$
$$\frac{1}{864}Q[1]^2\,Q[\{ei[1]\}]^2+\frac{Ft[2,ei[1],ei[2]]\,Q[1]\,Q[\{ei[1]\}]\,Q[\{ei[2]\}]}{1080}-$$
$$\frac{1}{288}Q\,Q[\{ei[1]\}]^2\,Q[\{ei[2]\}]^2-\frac{1}{540}Q^3\,Ft[2,ei[1],ei[2]]\,Q[\{ei[1],ei[2]\}]+$$
$$\frac{Q\,Ft[2]\,Ft[2,ei[1],ei[2]]\,Q[\{ei[1],ei[2]\}]}{2160}+$$
$$\frac{Q\,Ft[4,ei[1],ei[2]]\,Q[\{ei[1],ei[2]\}]}{1890}+\frac{Q\,Ft[2,ei[1],ei[2]]\,Q[1]\,Q[\{ei[1],ei[2]\}]}{1080}-$$
$$\frac{1}{120}Q^2\,Q[\{ei[1]\}]\,Q[\{ei[2]\}]\,Q[\{ei[1],ei[2]\}]+$$
$$\frac{1}{360}Q[1]\,Q[\{ei[1]\}]\,Q[\{ei[2]\}]\,Q[\{ei[1],ei[2]\}]-$$
$$\frac{1}{540}Q^3\,Q[\{ei[1],ei[2]\}]^2+\frac{1}{540}Q\,Q[1]\,Q[\{ei[1],ei[2]\}]^2+$$
$$\frac{1}{840}Ft[2,ei[1],ei[2]]\,Q[\{ei[2]\}]\,Q[\{ei[3]\}]\,Q[\{ei[1],ei[3]\}]-$$
$$\frac{1}{15\,120}Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[2]\}]\,Q[\{ei[4]\}]\,Q[\{ei[1],ei[3]\}]+$$
$$\frac{1}{15\,120}Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[2]\}]\,Q[\{ei[3]\}]\,Q[\{ei[1],ei[4]\}]+$$
$$\frac{1}{840}Ft[2,ei[1],ei[2]]\,Q[\{ei[1]\}]\,Q[\{ei[3]\}]\,Q[\{ei[2],ei[3]\}]+$$
$$\frac{1}{15\,120}Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[1]\}]\,Q[\{ei[4]\}]\,Q[\{ei[2],ei[3]\}]+$$
$$\frac{13\,Q\,Ft[2,ei[1],ei[2]]\,Q[\{ei[1],ei[3]\}]\,Q[\{ei[2],ei[3]\}]}{7560}+$$
$$\frac{17\,Q[\{ei[1]\}]\,Q[\{ei[2]\}]\,Q[\{ei[1],ei[3]\}]\,Q[\{ei[2],ei[3]\}]}{5040}+$$
$$\frac{4\,Q\,Q[\{ei[1],ei[2]\}]\,Q[\{ei[1],ei[3]\}]\,Q[\{ei[2],ei[3]\}]}{2835}+$$
$$\frac{Q\,Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[1],ei[4]\}]\,Q[\{ei[2],ei[3]\}]}{5040}+$$
$$\frac{Q[\{ei[1]\}]^2\,Q[\{ei[2],ei[3]\}]^2}{1080}-$$
$$\frac{1}{15\,120}Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[1]\}]\,Q[\{ei[3]\}]\,Q[\{ei[2],ei[4]\}]-$$
$$\frac{Q\,Ft[1,ei[1],ei[2]]\,Ft[1,ei[3],ei[4]]\,Q[\{ei[1],ei[3]\}]\,Q[\{ei[2],ei[4]\}]}{5040}+$$

$$\frac{1}{420} Q\, \text{Ft}[2, \text{ei}[1], \text{ei}[2]]\, Q[\{\text{ei}[3]\}]\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}] +$$
$$\frac{1}{840} Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2]\}]\, Q[\{\text{ei}[3]\}]\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}] +$$
$$\frac{1}{210} Q\, Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2], \text{ei}[3]\}]\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}] +$$
$$\frac{Q^2\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}]^2}{1680} -$$
$$\frac{Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[\{\text{ei}[1], \text{ei}[3], \text{ei}[4]\}]\, Q[\{\text{ei}[2], \text{ei}[3], \text{ei}[4]\}]}{1512} -$$
$$\frac{Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[\{\text{ei}[3], \text{ei}[4]\}]\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3], \text{ei}[4]\}]}{2835} +$$
$$\frac{1}{180} Q\, Q[1]\, Q[\{\text{ei}[1]\}]\, Q[1, \{\text{ei}[1]\}] - \frac{391\, Q[2]\, Q[\{\text{ei}[1]\}]\, Q[1, \{\text{ei}[1]\}]}{453\,600} +$$
$$\frac{1}{840} Q\, \text{Ft}[2, \text{ei}[1], \text{ei}[2]]\, Q[\{\text{ei}[2]\}]\, Q[1, \{\text{ei}[1]\}] +$$
$$\frac{1}{720} Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2]\}]^2\, Q[1, \{\text{ei}[1]\}] + \frac{17\, Q^2\, Q[1, \{\text{ei}[1]\}]^2}{10\,080} +$$
$$\frac{1}{840} Q\, \text{Ft}[2, \text{ei}[1], \text{ei}[2]]\, Q[\{\text{ei}[1]\}]\, Q[1, \{\text{ei}[2]\}] +$$
$$\frac{1}{720} Q[\{\text{ei}[1]\}]^2\, Q[\{\text{ei}[2]\}]\, Q[1, \{\text{ei}[2]\}] +$$
$$\frac{17\, Q\, Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[1, \{\text{ei}[2]\}]}{2520} -$$
$$\frac{31\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[1, \{\text{ei}[1]\}]\, Q[1, \{\text{ei}[2]\}]}{45\,360} +$$
$$\frac{5\, Q^2\, \text{Ft}[2, \text{ei}[1], \text{ei}[2]]\, Q[1, \{\text{ei}[1], \text{ei}[2]\}]}{3024} +$$
$$\frac{1}{280} Q\, Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2]\}]\, Q[1, \{\text{ei}[1], \text{ei}[2]\}] +$$
$$\frac{1}{420} Q^2\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[1, \{\text{ei}[1], \text{ei}[2]\}] -$$
$$\frac{61\, Q[1]\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[1, \{\text{ei}[1], \text{ei}[2]\}]}{75\,600} -$$
$$\frac{26\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[\{\text{ei}[2], \text{ei}[3]\}]\, Q[1, \{\text{ei}[1], \text{ei}[3]\}]}{42\,525} -$$
$$\frac{13\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[\{\text{ei}[1], \text{ei}[3]\}]\, Q[1, \{\text{ei}[2], \text{ei}[3]\}]}{42\,525} -$$
$$\frac{13\, Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}]\, Q[1, \{\text{ei}[2], \text{ei}[3]\}]}{12\,600} -$$
$$\frac{1}{945} Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2], \text{ei}[3]\}]\, Q[1, \{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}] -$$
$$\frac{2\, Q\, Q[\{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}]\, Q[1, \{\text{ei}[1], \text{ei}[2], \text{ei}[3]\}]}{4725} -$$
$$\frac{Q[1]\, Q[\{\text{ei}[1]\}]\, Q[2, \{\text{ei}[1]\}]}{1680} - \frac{Q\, Q[1, \{\text{ei}[1]\}]\, Q[2, \{\text{ei}[1]\}]}{4725} -$$
$$\frac{Q\, \text{Ft}[2, \text{ei}[1], \text{ei}[2]]\, Q[2, \{\text{ei}[1], \text{ei}[2]\}]}{7560} -$$
$$\frac{Q[\{\text{ei}[1]\}]\, Q[\{\text{ei}[2]\}]\, Q[2, \{\text{ei}[1], \text{ei}[2]\}]}{2520} - \frac{Q\, Q[\{\text{ei}[1], \text{ei}[2]\}]\, Q[2, \{\text{ei}[1], \text{ei}[2]\}]}{1890}$$

Appendix D

Mathematica Code: Wave Invariants

This Appendix contains the MATHEMATICA notebook used to compute the higher (partial) wave invariants. The notebook requires the computer algebra system MATHEMATICA [MMA15]. An introduction to MATHEMATICA can be found in [MMA08].

The notebook is avialable in digital form [Ber18].

Before providing the MATHEMATICA notebook two simplifications involved in the computation of wave invariants are given.

D.1 Simplify n

The wave invariants can be expressed more succinctly if we use the product

$$n_{i,j} \coloneqq \prod_{h=0}^{(j-i)/2} n-(i+2h) = (n-i)\cdot(n-(i+2))\cdots(n-j)\,,$$

where $i<j$ are two odd integers. For example,

$$n_{1,7} = (n-1)(n-3)(n-5)(n-7)\,.$$

The following Lemma gives an algorithm that extracts those integers i and j from a given polynomial.

Lemma D.1. If $i<j$ are two odd integers then

$$n_{i,j} = C_0 + C_1\cdot n^1 + \cdots + C_{k-1}n^{k-1} + n^k$$

implies that

$$i = 1-k-\frac{C_{k-1}}{k} \qquad \text{and} \qquad j = k-1-\frac{C_{k-1}}{k}\,.$$

Proof. It is clear that the maximal exponent k determines the number of factors in $n_{i,j}$ and that

$$k = \frac{j-i}{2} + 1\,.$$

On the other hand,

$$C_{k-1} = \sum_{h=0}^{(j-i)/2} -(i+2h) = \sum_{h=0}^{k-1} -(i+2h) = -ki - 2\frac{k(k-1)}{2}$$

such that

$$i = -(k-1) - \frac{C_{k-1}}{k} = 1 - k - \frac{C_{k-1}}{k}\,.$$

Since $j = 2(k-1) + i$ it follows that

$$j = 2(k-1) + 1 - k - \frac{C_{k-1}}{k} = k - 1 - \frac{C_{k-1}}{k}\,. \qquad \square$$

Remark D.2. In the MATHEMATICA script we have nonnormalized polynomials and it is generally not known whether $\frac{C_{k-1}}{kC_k}$ is an integer or not. We must test for this property and we cannot apply Lemma D.1 if this fraction is not an integer. However, in the first five wave invariants we always have $\frac{C_{k-1}}{kC_k} \in \mathbb{Z}$.

D.2 Fifth Wave Invariant

All small partial wave invariants can be computed using the MATHEMATICA notebook of Appendix D but the fifth small partial wave invariant can be simplified a bit further manually. Those simplifications are given in this Appendix.

Instead of giving the entire fifth invariant we shall instead study only those parts that are actually changed manually. The resulting invariant can be found in Theorem 5.8.

For example, the Q_{-Fl}-terms of $\mathsf{wi}_{5,l}(Q)$ are

$$\frac{5}{20736} Q_{-Fl} \tilde{F}_2(l,l)^4 - \frac{1}{18} Q_{-Fl} \tilde{F}_2(l,l) \tilde{F}_4(l,l)$$

and they can be simplified to

$$\frac{Q_{-Fl}}{18} |\tilde{F}l|^2 \Big(\frac{5}{1152} |\tilde{F}l|^6 - \tilde{F}_4(l,l) \Big),$$

because $\tilde{F}_2(l,l) = \tilde{F}(l,e_i)\tilde{F}(e_i,l) = -\tilde{F}(l,e_i)^2 = |\tilde{F}l|^2$.

Further, we can use the information contained within the case $l[c_1, c_2, -c_1 - c_2]$ and the multiindex notation of Definition 5.7 to rewrite the corresponding Q-sum:

$$\sum_{c\in l[c_1,c_2,-c_1-c_2]}^{Q} \frac{160}{\tilde{c}_1(l)^2\tilde{c}_2(l)^2(\tilde{c}_1(l)+\tilde{c}_2(l))^2}\tilde{c}_{1,3}\Big(\tilde{c}_1(l)^2\tilde{c}_{1,2}+\tilde{c}_2(l)\Big(\tilde{c}_1(l)+\tilde{c}_2(l)\Big)\tilde{c}_{2,3}\Big)$$
$$= \sum_{c\in l[c_1,c_2,-c_1-c_2]}^{Q} \frac{160}{\tilde{c}(l)^{(2,2,2)}}\tilde{c}_{1,3}\Big(\tilde{c}_1(l)^2\tilde{c}_{1,2}-\tilde{c}_2(l)\tilde{c}_3(l)\tilde{c}_{2,3}\Big)$$

Additionally, we can apply the permutation $p\colon l[c_1, c_2, -c_1 - c_2] \ni c \mapsto (c_2, c_3, c_1) \in l[c_1, c_2, -c_1 - c_2]$ to the second summand. The Q-sum simplifies to

$$\sum_{c\in l[c_1,c_2,-c_1-c_2]}^{Q} \frac{160}{\tilde{c}(l)^{(1,2,2)}}\tilde{c}_{1,2}\tilde{c}_{1,3}\Big(2\tilde{c}_1(l)+\tilde{c}_2(l)\Big).$$

Finally, the following two Lemmata will give a simplification of the sum of the Q-sums of the cases $l[c_1, -c_1, c_1, -c_1]$, $l[c_1, -c_1, c_3, -c_3]$ and $l[c_1, c_2, -c_2, -c_1]$. This sum, as computed by the MATHEMATICA notebook, has the following form:

$$\sum_{c\in l[c_1,-c_1,c_1,-c_1]}^{Q} \frac{-5}{|l|^2\tilde{c}_1(l)^4}\Big(\tilde{c}_1(l)^2\Big(3n_{9,11}+4|l|^2\Big(\tilde{c}_{1,1}+\tilde{c}_{1,2}\Big)\Big)+48|l|^2\Big(4\tilde{c}_{1,2}+\tilde{c}_{1,3}\Big)\Big)$$
$$+\sum_{c\in l[c_1,-c_1,c_3,-c_3]}^{Q} \frac{-5}{|l|^2\tilde{c}_1(l)^3\tilde{c}_3(l)^3}\cdot\Big($$
$$24|l|^2\tilde{c}_1(l)\tilde{c}_3(l)\Big(2\tilde{c}_{1,2}+\tilde{c}_{1,4}\Big)+24|l|^2\tilde{c}_3(l)^2\Big(6\tilde{c}_{1,2}+\tilde{c}_{1,3}+\tilde{c}_{1,4}\Big)$$
$$+\tilde{c}_1(l)^2\Big(\tilde{c}_3(l)^2\Big(3n_{9,11}+4|l|^2\Big(\tilde{c}_{1,1}+\tilde{c}_{1,2}\Big)\Big)+24|l|^2\Big(\tilde{c}_{1,3}+\tilde{c}_{1,4}\Big)\Big)\Big)$$
$$+\sum_{c\in l[c_1,c_2,-c_2,-c_1]}^{Q} \frac{120}{\tilde{c}_1(l)^3\tilde{c}_2(l)^3(\tilde{c}_1(l)+\tilde{c}_2(l))^2}\Big($$
$$\tilde{c}_1(l)^4\Big(\tilde{c}_{1,2}+\tilde{c}_{1,3}\Big)+\tilde{c}_2(l)^4\Big(\tilde{c}_{1,2}+\tilde{c}_{1,3}\Big)$$
$$+\tilde{c}_1(l)\tilde{c}_2(l)^3\Big(\tilde{c}_{1,2}+2\tilde{c}_{1,3}\Big)+\tilde{c}_1(l)^3\tilde{c}_2(l)\Big(\tilde{c}_{1,2}+2\Big(\tilde{c}_{1,3}+\tilde{c}_{1,4}\Big)\Big)\Big)$$

Lemma D.3. The following sums of the fifth partial wave invariant cancel for all choices of lattice $\mathcal{L}$, lattice vector $l \in \mathcal{L}\backslash\{0\}$ and potential Q.

$$0 = \sum_{c\in l[c_1,-c_1,c_1,-c_1]}^{Q} \frac{-5}{|l|^2\tilde{c}_1(l)^2}\Big(3n_{9,11}+4|l|^2(\tilde{c}_{1,1}+\tilde{c}_{1,2})\Big)$$
$$+\sum_{c\in l[c_1,-c_1,c_3,-c_3]}^{Q} \frac{-5}{|l|^2\tilde{c}_1(l)\tilde{c}_3(l)}\Big(3n_{9,11}+4|l|^2(\tilde{c}_{1,1}+\tilde{c}_{1,2})\Big)$$

Proof. Both sums actually have the same summand $s(c)$ and if we define

$$\pi c \coloneqq (c_1, c_2, c_4, c_3)$$

then $s(\pi c) = -s(c)$ for all $c \in l[c_1, -c_1, c_1, -c_1] \cup l[c_1, -c_1, c_3, -c_3]$. Further, π maps $l[c_1, -c_1, c_1, -c_1]$ bijectively onto a subset $C_0 \subset l[c_1, -c_1, c_3, -c_3]$ and hence

$$\sum_{c \in l[c_1,-c_1,c_1,-c_1]} s(c) + \sum_{c \in C_0} s(c) = \sum_{c \in l[c_1,-c_1,c_1,-c_1]} (s(c) + s(\pi c)) = 0\,.$$

On the other hand, the complement C_1 of C_0 in $l[c_1, -c_1, c_3, -c_3]$ is given by

$$C_1 \coloneqq l[c_1, -c_1, c_3, -c_3] \backslash \pi l[c_1, -c_1, c_1, -c_1] = \left\{ c \in \mathcal{L}'^4 \mid (c_2 + c_4)(l) \neq 0 \right\}$$

and thus π is a bijection of C_1 onto itself. Therefore,

$$\sum_{c \in C_1} s(c) = \frac{1}{2} \sum_{c \in C_1} (s(c) + s(\pi c)) = 0\,.$$

□

Lemma D.4. After applying Lemma D.3 to the fifth partial wave invariant we can merge the Q-sums of $l[c_1, -c_1, c_3, -c_3]$ and $l[c_1, c_2, -c_2, -c_1]$ as follows:

$$\begin{aligned}
&\sum_{c \in l[c_1,-c_1,c_3,-c_3]} s_1(c) + \sum_{c \in l[c_1,c_2,-c_2,-c_1]} s_2(c) \\
&= \sum_{c \in l[c_1,c_2,-c_2,-c_1]}^{Q} \frac{240}{\tilde{c}_1(l)\tilde{c}_2(l)^3(\tilde{c}_1 + \tilde{c}_2)(l)^2} \\
&\qquad \cdot \Big(\tilde{c}_1(l)^2(2\tilde{c}_{1,2} + \tilde{c}_{1,3} + 3\tilde{c}_{2,3} + \tilde{c}_{2,4}) \\
&\qquad + \tilde{c}_1(l)\tilde{c}_2(l)(2\tilde{c}_{1,2} + 2\tilde{c}_{1,3} + 5\tilde{c}_{2,3} + 2\tilde{c}_{2,4}) \\
&\qquad + \tilde{c}_2(l)^2(\tilde{c}_{1,3} + \tilde{c}_{1,4}) \Big)
\end{aligned}$$

Proof. It is easy to check that the map

$$p\colon l[c_1, c_2, -c_2, -c_1] \ni c \mapsto (c_1, c_4, c_3, c_2) \in l[c_1, -c_1, c_3, -c_3]$$

is well-defined and is its own inverse. We have

$$\sum_{c \in l[c_1,-c_1,c_3,-c_3]} s_1(c) + \sum_{c \in l[c_1,c_2,-c_2,-c_1]} s_2(c) = \sum_{c \in l[c_1,c_2,-c_2,-c_1]} (s_1(pc) + s_2(c))\,.$$

However, this does not, yet, give the expression above. We additionally use the permutation $c \mapsto (c_2, c_1, c_4, c_3)$ on $l[c_1, c_2, -c_2, -c_1]$ to obtain the expression for the merged Q-sum above. □

Wave Invariants

by Tillmann Berg

In this *Mathematica* notebook the first five (partial) wave invariants of Schrödinger operators on nondegenerate line bundles over even dimensional flat tori will be given. The calculation uses the procedure described in Section 4.4.

The results, the code and the explanations thereof can be accessed by double-clicking on the cell-brackets on the right hand side of this notebook. Pressing `Shift-Enter` within an `Input Cell` will execute this cell. Upon executing this notebook *Mathematica* will ask, for security reasons, whether it is allowed to execute the so-called `Initialization Cells`. Allowing *Mathematica* to do so is required as these cells contain the definitions used to construct the following function.

`WI[`k`]`

computes the kth partial wave invariant $\mathrm{WI}_{k,l}(Q)$ for fixed lattice vector l and potential Q.

Warning: The memory requirement for the computation of the wave invariants grows rapidly with the index of the invariants. Running those computations on a computer with insufficient memory may cause *Mathematica* and possibly other programs to freeze or crash and may cause a loss of data.

This *Mathematica* notebook was developed for *Mathematica* 10.3.1.0.

This notebook consists of five sections. In the first section we construct various functions needed to define the functions $H(i,j,k)$. After that we introduce various simplifications, in particular the τ-integration, used to reduce the size of the expressions. In the third section we define the wave invariants and show some properties thereof. The fourth section contains the computed partial wave invariants and the small partial wave invariants. The last section contains some miscellaneous computations. The results of the computation, the (small) partial wave invariants, can be found in the corresponding section below.

0.1 Notation

In this *Mathematica* notebook we implement a computation that follows the algorithm suggested by Section 4.4. To implement this recipe we need to represent several mathematical objects appearing in this section by *Mathematica* symbols. A list of some of those symbols and their meanings is given here. The symbols that are given here all have the property that they do not evaluate to another expression: They form the atomic building blocks of the symbolic analysis implemented in this *Mathematica* notebook.

`n`
: is any even and positive integer that represents the dimension of the flat torus M under consideration here.

`t`
: is a real number.

`tau[i]`
: represents τ_i, an integration variable integrated from 0 to 1.

The symbols `x`, `l`, `omega`, `Wi[_]`, `W` and `ei[_]` all represent vectors in $\mathbb{R}^n$. Other symbols have values in $\mathbb{R}$ or $\mathbb{C}$.

`x`
: is an element of $\mathbb{R}^n$ and represents a point in the flat torus.

`l`
: is some fixed nonzero lattice vector.

`nl`
: denotes the norm of the lattice vector `l`.

The following three symbols correspond to the smooth functions defined on $\mathbb{R}^{n-1}$ given in Section 4.4 and whose derivatives are given in
Theorem A.6.

`omega`
: represents the smooth function $\omega : \mathbb{R}^{n-1} \to \mathbb{R}^n$.

`omegal`
: denotes the scalar product $\langle \omega, l \rangle$ of `omega` with the lattice vector `l`. It is a smooth function $\mathbb{R}^{n-1} \to \mathbb{R}^n$.

`v`
: denotes the smooth function $v : \mathbb{R}^{n-1} \to \mathbb{R}$.

There are two orthonormal bases for $\mathbb{R}^n$: the standard basis e_i and the vectors W_i that form an orthonormal basis together with the normalized lattice vector `l/nl`. Both basis generally occur with several distinct indices within expressions and we therefore have to

distinguish those indices. It is assumed that indices are summed over.

`Wi[h]`
: represents the vector W_{i_h} and each such index is summed over from `1` to `n-1`.

`W`
: represents the only vector `Wi` that can appear if we compute the wave invariants in dimension `2`.

`ei[h]`
: denotes the standard basis vector e_{i_h}. Here the indices are summed over `1` to `n`.

Further, we need the forms originating from the given connection and its curvature. Recall, that a tilde over any symbol abbreviates a factor $2\pi i$ and this tilde is represented here by adding the letter `t` to the letter symbolising the mathematical object.

`AD[X, Y]`
: represents the connection 1-form $A^D_X(Y)$ of the distinguished connection.

`at[Y]`
: represents $\tilde{a}(Y) = 2\pi i a(Y)$, the 1-form parametrising connections.

`Ft[X, Y]`
: denotes the curvature $\tilde{F}(X, Y)$ of the connection times the factor $2\pi i$.

The potential `Q` of our Schrödinger operator has not one but two arguments. The second argument gives a (possibly empty) `List` of vectors in whose direction the potential is differentiated and the first argument gives the point at which this derivative of the potential is evaluated.

`Q[X, der]`
: the potential `Q` at the point X with the derivatives in the (possibly empty) `List` *der* applied.

We also need to expand this potential into its Fourier series. Two types of Fourier coefficients appear:

`QmFl`
: is the Fourier coefficient Q_{-Fl} of Q with the index *-F(l)*.

`SumQ[case, exp]`
: is a Q-sum of *exp* over the integrated or unintegrated *case*.

`Case[c1, c2, ...]` or `l[c1, c2, ...]`
: denote the integrated and unintegrated cases of varying length.

The children of the cases have varying form in this notebook for technical reasons. Its

elements are denoted similarly to `at`.

`ct[i, Y]`
: represents the ith component $\tilde{c}_i(Y) = 2\pi i c_i(Y)$ of an element of a case applied to the vector Y.

`ctl[alpha]`
: does not evaluate and denotes $\tilde{c}_{l_1}(l)^{\alpha_1} \cdots \tilde{c}_{l_k}(l)^{\alpha_k}$, where k is the length of the sequence $alpha$.

There are some other atomic symbols which only appear as intermediate symbols and are omitted here. To formulate the results some further symbols are needed. There are variations of the notation for the dimension `n` and the curvature form `Ft`.

`n[i,j]`
: represents the $n_{i,j} = \prod_{h=0}^{(j-i)/2} n-(i+2h)$ defined in Section D.1.

`Ft[k,X,Y]` and `Ft[k]`
: are curvature traces defined in Definition 3.7.

`Trct[i,j]` and `TrctSq`
: denote certain (sums of) traces over bilinear maps of the form $\tilde{c}_i\,\tilde{c}_j$ given in Definition 5.3.

1 Definitions for Creation

1.1 Tests

In the construction of the wave invariants several test functions are needed. The following function is merely the negation of `FreeQ`.

`ContainsQ[exp, pat]`
: yields `True` if the pattern pat is contained in the expression exp, and yields `False` otherwise.

```
ContainsQ[exp_, pat_] := Not@FreeQ[exp, pat]
```

The following function is merely an abbreviation.

FreexQ[*exp*]
yields True if the expression *exp* is free of the variable x, and yields False otherwise.

```
FreexQ[exp_] := FreeQ[exp, x]
```

Further, we are going to define multilinear functions on $\mathbb{R}^n$. This linearity should not just apply with respect to Plus but we also need to pull-out scalar factors. For this we need *Mathematica* to distinguish between scalars and vectors. The following symbols and expressions are understood as vectors in $\mathbb{R}^n$: omega, l, x, ei[_], Wi[_] and W. Everything not a vector is considered a scalar.

CVectorQ[*arg*]
yields True if the argument *arg* is vector and False otherwise.

The "C" stands for "custom" and is used to distinguish this function from the different build-in function VectorQ, which we do not need. Note that this function and related constructs are independent of any choice of dimension. Thus, the differential operators defined below and the related analysis work in every dimension (with one exception discussed later).

```
CVectorQ[arg_] := MatchQ[arg, omega | l | x | ei[_] | Wi[_] | W]
```

Finally, we do need differentiations with respect to the z-variables. However, no z-variables will appear explicitly in any expression used to calculate the wave invariants. Instead, we define the following functions as z-dependent: v, omega and omegal.

FreezQ[*arg*]
yields True if the expression *exp* does not contain any functions of z. Otherwise, False is returned.

Note, that omega is understood as a vector-valued function depending on z and the definitions of FreezQ and CVectorQ are not inconsistent. omegal is understood as the scalar product of the vectors omega and l.

```
FreezQ[exp_] := FreeQ[exp, v | omega | omegal]
```

Examples

```
ContainsQ[Q[x], x]
```

```
True
```

```
FreexQ[Q[x]]
```

```
False
```

```
{CVectorQ[x], CVectorQ[omegal]}
```

```
{True, False}
```

Note that `FreezQ[exp]` would return `True` even if the expression *exp* contains `z`. This is not an issue as the variable `z` will not be used later. It will appear only implicitly in the form of `v`, `omega` and `omegal`.

```
{FreezQ[z], FreezQ[omega]}
```

```
{True, False}
```

1.2 Linearity

Having the test functions of the previous section at our disposal we can define the following multilinear functions on $\mathbb{R}^n$.

`AD[X,Y]`
: is a bilinear map.

`AD` is linear with respect to `Plus` in both arguments and scalars are distinguished from vectors using `CVectorQ` and pulled out. If one argument is zero then linearity defined in this way would not lead to `AD` vanishing. This needs to be defined explicitly.

```
AD[X1_ + X2_, Y_] := AD[X1, Y] + AD[X2, Y]
AD[X_, Y1_ + Y2_] := AD[X, Y1] + AD[X, Y2]
AD[alpha_ * X_?CVectorQ, Y_] := alpha * AD[X, Y]
AD[X_, alpha_ * Y_?CVectorQ] := alpha * AD[X, Y]
AD[0, _] := 0
AD[_, 0] := 0
```

The following map has only one argument and is set to be linear in the same fashion.

`at[X]`
: is a linear map.

```
at[X_ + Y_] := at[X] + at[Y]
at[alpha_ * X_?CVectorQ] := alpha * at[X]
at[0] := 0
```

The sum of AD and at gives the connection form.

A[X, Y]
: is the bilinear connection form.

```
A[X_, Y_] = AD[X, Y] + at[Y];
```

Besides the linearity of the connection form we also need linearity in the derivatives of the potential Q.

Q[X, der]
: represents the potential Q at the point X with the derivatives in the (possibly empty) List der applied. Q[X, der] does not evaluate but is linear in every element of der.

For example, Q[X, {}] represent the potential Q at the point X, while Q[X, {V}] represents the gradient of Q at the point X times the vector V and Q[X, {V,W}] represents the Hessian of Q at X paired with the vectors V and W.

```
Q[X_, {der1___, V1_ + V2_, der2___}] :=
 Q[X, {der1, V1, der2}] + Q[X, {der1, V2, der2}]
Q[X_, {der1___, alpha_ * V_?CVectorQ, der2___}] :=
 alpha * Q[X, {der1, V, der2}]
Q[_, {___, 0, ___}] := 0
```

The pattern der1___ returns a Sequence of arbitrary length, including the empty sequence. For example,

```
Q[x, {V1 + V2, V3, V4}]
```

```
Q[x, {V1, V3, V4}] + Q[x, {V2, V3, V4}]
```

1.3 Derivatives

In the construction of the wave invariants three types of derivatives are involved: Those

with respect to t, x and z.

Derivation with respect to t

Let us define the derivative with respect to t first.

dt[*exp*]
returns the derivative of *exp* with respect to t.

If *exp* is free of t then the derivative vanishes and the derivative of t by t is 1. The third line gives linearity of dt and the fourth the Leibniz rule.

```
dt[exp_ /; FreeQ[exp, t]] := 0
dt[t] := 1
dt[exp_Plus] := dt /@ exp
dt[a_ * b_] := dt[a] * b + a * dt[b]
```

If *exp* is an exponentiation then it is clear from the construction of the wave invariants that the exponent is an integer and, in particular, free of t. Also, the exponential function Exp is needed. Its derivative can be set explicitely.

```
dt[a_^b_] := b * a^(b - 1) * dt[a]
dt[Exp[a_]] := Exp[a] * dt[a]
```

Finally, we need to define how the potentials Q are to be differentiated with respect to t. In principle, both the argument *X* of Q[*X*, *der*] and the elements of the List of derivatives *der* may depend on t. However, t is not a vector (according to CVectorQ) and the linearity of Q with respect to the elements of *der* will ensure that all t are pulled out of Q. Thus, only *X* may depend on t and we can simply apply the chain rule.

```
dt[Q[X_, der_]] := Q[X, Append[der, dt@X]]
```

Analogously, the linearity of AD and at guarantee that their arguments are free of t. There is no need to define a derivation of those functions with respect to t.

Derivation with respect to x

Secondly, let us define the derivative with respect to x.

`dxi[k, exp]`
returns the derivative of exp with respect to the variable x_{i_k}.

Caveat: `dxi[k, exp]` does *not* represent the derivative of exp with respect to the variable x_k.

The derivation with respect to `x` works generally in the same way as the derivation with respect to `t`, except that we have to take account of which of the variables x_1 to x_n is meant when differentiating. However, in the construction of the wave invariants only sums over pairs of standard vectors e_i and standard coordinates x_i appear, where the index i of those sums ranges from 1 to n. Thus, we will add an index k to each derivation but this index enumerates the indices i_k in our expressions, where each of the indices i_k is summed over from 1 to n.

The advantage of this approach is that we obtain a calculus that is independent of the dimension n. Note that the derivation of `x` with respect to the index of indices k is, of course, not 1 but the standard vector e_{i_k}.

```
dxi[k_, _?FreexQ] := 0
dxi[k_, x] := ei[k]
dxi[k_, exp_Plus] := dxi[k, #] & /@ exp
dxi[k_, a_ * b_] := dxi[k, a] * b + a * dxi[k, b]
dxi[k_, a_^b_] := b * a^(b - 1) * dxi[k, a]
dxi[k_, Exp[a_]] := Exp[a] * dxi[k, a]
```

Since `x` is a vector, the functions `AD` and `at` may depend on `x`. However, from the construction of the wave invariants it is clear that in `AD[a, b]` only a can contain an `x`. The linearity guarantees that if a contains an `x` it must be exactly `x`. `at[b]` cannot depend on `x`. Therefore, it is sufficient to define the following derivation rule.

```
dxi[k_, AD[x, b_]] := AD[ei[k], b]
```

Finally, we need to define a `dx`-derivation for the potential `Q`. By Lemma B.3 the derivatives in der are free of `x` and the derivative of the argument X with respect to x_{i_k} is the standard basis vector e_{i_k}.

```
dxi[k_, Q[X_, der_]] := Q[X, Append[der, ei[k]]]
```

Derivation with respect to z

Analogously to the derivation with respect to `x` we define a derivation with respect to `z`:

`dzi[k, exp]`
returns the derivative of *exp* with respect to the variable z_{i_k}.

Again, we have to keep track of the indices in use. There is one less `z`-variable than `x`-variables and thus the indices of the `z`-variables are summed over from *1* to *n-1*. This difference in the summation need not be encoded, however.

```
dzi[k_, _?FreezQ] := 0
dzi[k_, exp_Plus] := dzi[k, #] & /@ exp
dzi[k_, a_ * b_] := dzi[k, a] * b + a * dzi[k, b]
dzi[k_, a_^b_] := b * a^(b - 1) * dzi[k, a]
dzi[k_, Exp[a_]] := Exp[a] * dzi[k, a]
```

The symbol `z` does not appear in the computation of the wave invariants. The dependence on the corresponding variables is implicit in the functions `v`, `omega` and `omegal`. Here, in `AD[a, b]` both *a* and *b* may depend on `z`, because `omega` is a vector. Also, `at[b]` can depend on `z`. Bilinearity and linearity give the following derivation rules.

```
dzi[k_, AD[a_, b_]] := AD[dzi[k, a], b] + AD[a, dzi[k, b]]
dzi[k_, at[b_]] := at[dzi[k, b]]
```

In the case of `z`-derivatives not only the argument *X* of the potential but also every derivative in *der* may depend on `z`. The Leibniz rule gives the following derivative.

```
dzi[k_, Q[X_, der_]] :=
 Q[X, Append[der, dzi[k, X]]] +
  Sum[Q[X, MapAt[dzi[k, #] &, der, index]],
   {index, Length@der}]
```

Finally, it remains to calculate the `z`-derivatives of the functions `v`, `omega` and `omegal`. However, those derivatives are complicated and will be computed later. Thus, we just remember which derivatives have been applied.

`v[der]` and `omega[der]`
do not evaluate. *der* is a `List` of indices of indices of the `z`-derivatives that have been applied to `v` and `omega`.

```
dzi[k_, v[der_]] := v[Append[der, k]]
dzi[k_, omega[der_]] := omega[Append[der, k]]
```

The case of `omegal` is simpler. By Theorem A.6 only $\omega(0)l$ and $\partial_i \partial_i \omega(0)\, l$ do not vanish. Therefore, *der* does not need to be a `List` but merely the index of the first derivation of `omegal`. The second derivation can be computed explicitely at this point. We do not use lists of derivatives but denote the first derivative by `omegal[k]` and use the fact that all indices in the following `Sumzd` will be distinct for the second derivative.

```
dzi[k_, omegal] := omegal[k]
dzi[k_, omegal[der_]] := If[der == k, -nl, 0]
```

Recall that `nl` represents the norm of the nonzero lattice vector `l`.

Examples

The symbol `a[0]` is defined below as

```
a[0] = Exp[A[x + t * omega / 2, t * omega]];
```

and we can apply the three types of derivatives to this functions.

```
dt[a[0]]
```

$$e^{\frac{1}{2} t^2 \,\mathrm{AD[omega,omega]} + t\,\mathrm{AD[x,omega]} + t\,\mathrm{at[omega]}}$$

$$(t\,\mathrm{AD[omega,\ omega]} + \mathrm{AD[x,\ omega]} + \mathrm{at[omega]})$$

```
dxi[1, a[0]]
```

$$e^{\frac{1}{2} t^2 \,\mathrm{AD[omega,omega]} + t\,\mathrm{AD[x,omega]} + t\,\mathrm{at[omega]}}\ t\,\mathrm{AD[ei[1],\ omega]}$$

If we are to derive with respect to `z` then `omega` needs to be replaced by `omega[{}]`.

```
dzi[1, a[0] /. omega → omega[{}]]
```

$$e^{t\,\mathrm{AD}[x,\mathrm{omega}[\{\}]]+\frac{1}{2}t^2\,\mathrm{AD}[\mathrm{omega}[\{\}],\mathrm{omega}[\{\}]]+t\,\mathrm{at}[\mathrm{omega}[\{\}]]}$$
$$\left(t\,\mathrm{AD}[x,\ \mathrm{omega}[\{1\}]]+\frac{1}{2}t^2\,(\mathrm{AD}[\mathrm{omega}[\{\}],\ \mathrm{omega}[\{1\}]]+\mathrm{AD}[\mathrm{omega}[\{1\}],\ \mathrm{omega}[\{\}]])+t\,\mathrm{at}[\mathrm{omega}[\{1\}]]\right)$$

1.4 Defining a_i

After having defined derivations we can now proceed to define the following symbols.

`a[i]`
: returns the ith symbol of the approximate wave kernel.

In fact, we will define two versions of those symbols. The definition of `a[i]` simply follows Section 4.4. However, by the necessary conditions of Section 4.6 we know that the wave invariants must be free of `at` and that each summand of the wave invariants must contain the potential `Q`. This can be used to drop unneeded summands early on in the computation, resulting in a reduction of the time and memory requirements of the computation by around a factor of seven.

`aQ[i]`
: returns the ith symbol of the approximate wave kernel with `at` set to zero and such that every term contains the potential `Q`.

The original definition can be used to test the correctness of the computation.

Slow Definition

We will start with the simpler but slower definition.

`box[k, exp]`
: applies the box operator (in standard coordinates) to the expression exp using the index i_k for sums, see Definition 4.9.

```
box[k_, exp_] := dt[dt[exp]] - dxi[k, dxi[k, exp]] -
  AD[ei[k], ei[k]] * exp - 2 * A[x, ei[k]] * dxi[k, exp] -
  A[x, ei[k]]^2 * exp + Q[x, {}] * exp
```

After applying the box operator we substitute the arguments according to Section 4.4.

`TauIntegrand[`i`,`exp`]`
divides by `a[0]` and substitutes the arguments in the `tau`-integrand exp.

The `Rule Exp[_]→1` implements the division by `a[0]`. Implementing this division in this way ensures that indeed all occurencies of `a[0]` are removed from the expression.

```
TauIntegrand[i_, exp_] :=
 exp /. {Exp[_] → 1, t -> tau[i] * t, x → x + (1 - tau[i]) * t * omega}
```

With the box operator and the substitution we can, inductively, define the symbols `a[`i`]`.

```
a[0] = Exp[A[x + t * omega / 2, t * omega]];
a[i_] := a[i] =
  SelectiveExpand[a[0] * I / 2 * t *
    TauIntegrand[i, box[2 * i, a[i - 1]]]]
```

Here, it is understood that, similarly to the Einstein convention for indices, the variables `tau[`i`]` are integrated over from `0` to `1`. It would be possible to compute some of those integrals at this point. However, for this we would need to expand `a[`i`]` via `Expand` and this would be more time and memory costly than computing those integrals later. So, we only selectively expand (some of) the arguments of the potentials within the `a[`i`]`.

```
SelectiveExpand[exp_] :=
 exp /. Q[xl_ /; Length@xl > 2, der_] :↦ Q[Expand@xl, der]
```

Note that the definition uses memoization. Also, in order to avoid variable conflicts between `dx`- and `ei`-indices on the one hand and `dz`-integrals on the other hand the box operator uses even indices only.

Fast Definition

For the faster definition we will change the definition of the `a[`i`]` in two ways: We will drop all occurrencies of `at` from the definition of `a[`i`]`, which means replacing all `A` by `AD`, and we split the box operator and the `a[`i`]` into one part that is free of the potenial `Q` and one part in which every summand contains the potential.

By the necessary condition of Lemma 4.41 all terms containing `AD[x,_]` must cancel as well. But since computing the $(i+1)$th symbol involves `dx`-derivatives of the ith symbol we cannot simply remove the `AD[x,_]` at this point of the computation of the wave

invariants. It will be done later.

The definition of the box operator follows those of the slow version box, except that at and Q are set to zero.

boxNoQ[k,exp]
: applies the box operator (in standard coordinates) to the expression exp using the index i_k for sums. Terms containing at or Q are removed.

```
boxNoQ[k_, exp_] := dt[dt[exp]] - dxi[k, dxi[k, exp]] -
  AD[ei[k], ei[k]] * exp - 2 * AD[x, ei[k]] * dxi[k, exp] -
  AD[x, ei[k]]^2 * exp
```

Again, we can use the box operator to define the symbols a[i] according to Section 4.4. However, this time we define two sets of symbols following Definition 4.47.

aQ[i] and aNoQ[i]
: added together constitute the ith symbol of the approximate wave kernel with at set to zero. aQ contains the terms with potential and aNoQ is free of the potential Q.

Again, this definition uses memoization and uses even indices to avoid variable conflicts. As before the symbols are only selectively expanded and no tau[i]-integrals are evaluated, even though it would be possible to compute some of them.

```
aNoQ[0] = Exp[AD[x + t * omega / 2, t * omega]];
aQ[0] = 0;

aNoQ[i_] := aNoQ[i] =
    aNoQ[0] * I / 2 * t *
     TauIntegrand[i, boxNoQ[2 * i, aNoQ[i - 1]]];
aQ[i_] := aQ[i] =
  SelectiveExpand[aNoQ[0] * I / 2 * t * TauIntegrand[i,
     boxNoQ[2 * i, aQ[i - 1]] + Q[x, {}] * (aQ[i - 1] + aNoQ[i - 1])
    ]]
```

The fast definition aQ[5] requires around 37 % less time and 63 % less memory to compute than a[5]. More importantly, aQ[5] is only half as big as a[5], which greatly increases the speed of the following computations and reduces their memory needs.

1.5 The z-Laplacian

In this section we define the Laplacian with respect to the z-variables evaluated at ***z=0***.

`Delta[k, exp]`
applies the z-Laplacian k times to the expression exp and evaluates the result at ***z=0***.

To compute the value of `omega[der]` and `v[der]` at `z=0` we use Theorem A.6. It is important to note that there is a difference between the derivatives α used in Theorem A.6 and the indices of indices der. In order to apply Theorem A.6 we need to assume that the indices indexed by der are distinct (if they do not have the same index and are identical) and construct the Laplacian correspondingly. Also, some z-derivatives lead to expressions that cease to contain indices. Thus, we cannot use the Einstein convention for those sums and the following definition is needed.

`Sumzd[indices, exp]`
does not evaluate. Denotes a sum of exp over the indices indexed by $indices$ from 1 to $n-1$ such that those indices are pairwise-distinct.

For example,

```
Sumzd[{3, 5}, AD[Wi[3], Wi[5]]];
```

represents to $\sum_{i_3 \neq i_5=1}^{n-1} \mathrm{AD}[W_{i_3}, W_{i_5}]$. Unfortunately, a dependence on the dimension n enters our computation at this point: Such a sum only exists if the dimension n is sufficiently large to accomodate the distinct indices. To accomodate k distinct z-variables the dimension needs to be at least $k+1$ and even.

For this reason, we need to perform different calculations for small dimensions. To set the dimension and compute the wave invariants accordingly we use the following functions.

`SetDimension[`*dim*`]`
: sets the dimension used in the computation of the wave invariants to *dim*, which can either be some numerical value (positive even integer) or `Large`. If `Large` is given instead of a numerical argument then it will be assumed that the dimension is as large as needed. The default setting is `Large`.

`DimensionQ[`*dim*`]`
: returns `True` if the dimension set using `SetDimension` is greater or equal to *dim* and `False` if it is less then *dim*.

Implementation

Let us start the definition of `SetDimension` with the case that a numerical value is given for the dimension.

```
SetDimension[dim_] := (
  DimensionNQ = True;
  (* A numerical value is given for the dimension. *)
  dimension = dim;    (* Save this value. *)
  Clear@DimensionQ;  (* Delete previous definitions. *)
  DimensionQ[_] := True;
  DimensionQ[k_ /; k > dim] := False;
 )
```

Setting the dimension to `Large` is supposed to mean that `DimensionQ[`*dim*`]` is `True` for all dimensions *dim*, i.e. the dimension is large enough to accomodate all `z`-indices in the computation of a wave invariant. Since the computation of any wave invariant involves only finitely many `z`-indices this definition is meaningful. Of course, what dimensions can be considered `Large` depends on which wave invariant we are computing.

```
SetDimension[Large] := (
  DimensionNQ = False;
  (* No numerical value is given for the dimension. *)
  dimension = Large;    (* Save this setting anyway. *)
  Clear@DimensionQ;
  (* If the dimension is set to Large it is assumed
   to be always larger than any given argument of
   DimensionQ. *)
  DimensionQ[_] := True
 )
```

Finally, we set the `Large` case as the default setting. It will turn out later that at least for the first five wave invariants the invariants for smaller dimensions are equal to the wave invariant with the dimension set to `Large`.

```
SetDimension[Large]
```

In the case `n=2` one might be tempted to set `Wi[_]:=W`. However, this conflicts with the memoization of, for example, `omega0.` If `omega0` were computed in dimension 2 with this simplification and then used later for higher dimensions, it would still contain the, then incorrect, simplification `Wi→W`. Similarly, we cannot set `n→dimension`. Those substitutions can be performed later and for this purpose the dimension is stored in `dimension` and `DimensionNQ` is `True` exactly if a numerical value for the dimension is given.

Now, the `z`-Laplacian is defined as follows.

```
Delta[0, exp_] := EvaluateAtz0@exp
Delta[k_, exp_] :=
 EvaluateAtz0[Plus @@ (MakeSumzd[#, exp] & /@ Partitions@k)]
```

Here `EvaluateAtz0` evaluates the three functions `omega`, `omega1` and `v` and their derivatives at `z=0`. If zero Laplacians are applied only this functions is needed. If k Laplacians are applied we want to generate only sums whose indices are distinct. Thus, we compute all `Partitions` of k and for each partition we generate such a sum (with correct multiplicity), see Theorem A.9.

MakeSumzd[*partition*, *exp*]
: generates the part of the k z-Laplacians applied to *exp* that corresponds to the *partition*.

First, we have to check whether the dimension currently set by SetDimension is sufficiently large to accomodate the distinct indices. If it is not the sum must vanish.

```
MakeSumzd[partition_, exp_] :=
 If[DimensionQ@EvenInteger[Length@partition + 1],
  (* Dimension is sufficiently large *)
     MakeSumzd[2 * Range@Length@partition + 1, partition,
   exp],
  (* Dimension is to small *)
     0
 ]
```

To prevent variable collisions between the indices of Wi and ei, the z-derivatives and therefore later the vectors Wi only use odd *indices*.

The dimension has to be both strictly larger than the number of indices Length@*partition* and even. EvenInteger[*i*] gives the smallest even integer that it is greater or equal to *i*.

```
EvenInteger[i_] := If[EvenQ@i, i, i + 1]
```

MakeSumzd[*indices*, *partition*, *exp*]
: computes the z-derivatives denoted by *indices* of *exp* as often as given by the *partition*. Also contains an integer factor giving the multiplicities of each sum such that the total sum gives the correct application of k z-Laplacians.

The integer factor giving the multiplicities is given by CMultinomial[*partition*], see Theorem A.9.

```
MakeSumzd[indices_, partition_, exp_] :=
 CMultinomial@partition *
  Sumzd[indices,
   Fold[dzi2k, exp, Transpose[{indices, partition}]]]

CMultinomial[partition_] :=
 (Multinomial @@ partition) /
  (Times @@ (Tally[partition][[All, 2]]!))
```

Here,

`dzi2k[exp,{index,k}]`
applies $2k$ `z`-derivatives to *exp* using the *index*.

At this point, we can already apply Theorem A.6 and set all those derivatives to zero that can already be seen to vanish. After completing all derivatives with respect to a given index the function `v` must vanish if it contains an odd number of derivatives with respect to this index. If the derivatives of `omega` contain more than one odd multiplicity then it must vanish, as well. This leads to a slightly slower but also less memory intensive computation.

```
dzi2k[exp_, {index_, k_}] :=
 Nest[dzi[index, dzi[index, #]] &, exp, k] /.
  {v[der_ /; OddQ@Count[der, index]] → 0,
   omega[der_ /; Length@OddDer@der > 1] → 0}
```

The `z`-derivatives of `omega` and `v` are only stored during differentiation and it remains to evaluate those derivatives at ***z=0***.

`EvaluateAtz0[exp]`
evaluates `omega`, `omegal` and `v` at `z=0`. Also, removes exponential terms.

Since no further derivatives have to be computed and since the form of the exponential terms is clear for all wave invariants we can remove those terms here.

```
EvaluateAtz0[exp_] :=
 exp /. {Exp[_] → 1, v → v0, omega → omega0, omegal[_] → 0,
   omegal → nl}
```

`v0[der]` and `omega0[der]`
evaluate the derivatives *der* of `omega` and `v` at ***z=0*** according to Theorem A.6.

```
v0[der_] := v0[der] = If[
    Or @@ OddQ@Tally[der][[All, 2]],
        0,
    Times @@ ((Tally[der][[All, 2]] - 1)!!) * 2^(-Length@der) *
     Product[1 - n + 2 * i, {i, Length@der / 2}]]
```

For the evaluation of `omega` we need the function `OddDer[der]` that collects those derivatives *der* with an odd multiplicity. If there is more than one such index `omega0[der]` must vanish. If there is exactly one such index *h* then `omega0[der]` is given by `Wi[h]` times some constant given by `calphai[der]`.

```
OddDer[der_] := Cases[Tally@der, {_, _?OddQ}]
calphai[der_] :=
 -2 *
  Times @@
   (Replace[Tally@der, {{_, c_?OddQ} → c, {_, c_} → c - 1},
      {1}]!!) * (Length@der - 4)!! * 2^(-Length@der)

omega0[{}] = 1 / nl;
omega0[{i_, i_}] = -1 / nl;
omega0[der_] := omega0[der] = If[
    Length@OddDer@der == 1,
        Wi[OddDer[der][[1, 1]]] * calphai@der,
    0]
```

This concludes the definition of the `z`-Laplacian and allows us to construct the wave invariants according to Section 4.4.

1.6 Definition of H

We now have all necessary definitions to construct the wave invariants according to Section 4.4. Recall that we have a slow and a fast definition of the `a[i]` and we need to

specify which one to use.

`SetSpeed[Speed]` and `SetSpeed[Thorough]`
: define whether the wave invariants should be computed quickly by using the necessary conditions or whether a more thorough computation should be performed to test the correctness of the computation of the wave invariants. By default the fast version is used.

```
SetSpeed[Speed] := (SpeedVar = True;)
SetSpeed[Thorough] := (SpeedVar = False;)
SetSpeed[Speed]
```

`H[{i,j,k}]`
: returns `H` for the k-th wave invariant and the summation indices i and j as defined in Section 4.4.

If `Speed` is set then `at` is set to zero and every summand must contain the potential `Q`. This is already contained in the fast version of the definition of `a[i]`. Also, all terms containing `AD[x,_]` must vanish and thus we can set `AD[x,_]` to zero (after having computed all `x`-derivatives).

```
H[{i_, j_, k_}] :=
 1 / j! * (-2 I nl)^(-j) Binomial[n - 1 - i, k - i - j]
  I^(k - i - j) Delta[j, v[{}] * arg@Nest[dt,
      If[SpeedVar,
       aQ[i] /. AD[x, V_] → AD[l, V], (* Speed *)
       a[i] (* Thorough *)
      ],
      k - i - j]]
```

Here, `arg[exp]` substitutes the arguments after computing the `t`-derivatives.

```
arg[exp_] := exp /. {t → omegal, x → x + l, omega → -omega[{}]}
```

The wave invariants are given as a sum of `H` over all nonnegative integers with $i+j \le k$.

`HIndices[k]`
generates the indices over which the `H` must be summed to obtain the k-th wave invariant.

```
HIndices[k_] := Join @@ Table[{i, j, k}, {j, 0, k}, {i, 0, k - j}]
```

For example,

```
HIndices[2]
```

```
{{2, 0, 0}, {2, 0, 1}, {2, 0, 2}, {2, 1, 0}, {2, 1, 1}, {2, 2, 0}}
```

We have already mentioned that the computation of the `z`-derivatives changes in lower dimensions and we can set the dimension of the current computation via `SetDimension`. It follows from the construction that the wave invariants only have to be computed separately for finitely many small dimensions and for large dimensions. More precisely, by Section 4.4 the computation of the kth wave invariant contains at most k `z`-Laplacians and thus at most k `z`-indices. For those indices to all be distinct the dimension needs to be at least $k+1$ and even. Any such dimension is subsumed in the `Large` dimension setting. The lower even dimensions have to be computed separately.

However, the highest number of `z`-derivatives appears only in the term `H[{0,k,k}]` and this term is free of the potential `Q`. If `SetSpeed` is set to `Speed` then this term always vanishes. In this case, the maximal number of distinct `z`-variables in any term is only `k-1` and thus the `Large` dimension case is reached with the first even integer greater than or equal to k.

The following function gives those dimensions that need to be computed seperately.

`NeededDimensions[k]`
returns a list of those dimensions one has to differentiate in the computation of the kth wave invariant.

```
NeededDimensions[k_] := If[SpeedVar,
  Append[Range[2, EvenInteger[k] - 2, 2], Large],
  Append[Range[2, EvenInteger[k + 1] - 2, 2], Large]
 ]
```

The different dimensions that need to be considered for the wave invariants are given by the following list.

```
SetSpeed[Speed]
{#, NeededDimensions@#} & /@ Range[7] // Column
```

```
{1, {Large}}
{2, {Large}}
{3, {2, Large}}
{4, {2, Large}}
{5, {2, 4, Large}}
{6, {2, 4, Large}}
{7, {2, 4, 6, Large}}
```

1.7 Example

Using the functions defined so far we can already compute the first partial wave invariant, which is the sum of the following three terms. The third term is zero, of course.

```
H /@ HIndices[1]
```

$$\left\{0,\ \frac{1}{2}\,\text{i nl Q}[\text{l} + \text{x} - \text{l}\,(1 - \text{tau}[1]),\ \{\}],\ \frac{\text{i Sumzd}[\{3\},\ 0]}{2\,\text{nl}}\right\}$$

However, the third partial wave invariant is already rather large.

```
ByteCount[Plus @@ H /@ HIndices[3]]
```

```
2 496 392
```

One might try to use the `Simplify` function to reduce the size of the third partial wave invariant. Due to the generality of this function this is rather slow (4 minutes) to compute and does not give a much smaller expression (1.8 MB in size). Also, `Simplify` cannot perfom `x`- or `tau`-integrations, since those are, of course, not known to *Mathematica.*

Hence, some simplifications are needed to reduce the size of those invariants and in the following section we shall define those. It will turn out that the third partial wave invariant can be computed in around 13 seconds and then requires only 3,472 bytes to store.

2 Definitions for Simplification

The goal of this section is to define functions that simplify the partial wave invariants obtained by using the function `H` defined in the previous section.

`SimplifyWI[exp]`
simplifies the expression *exp*.

In particular, we need to replace the sums with distinct indices `Sumzd` by conventional sums, substitute the vectors `ei` by the vectors `Wi` and `l/nl`, remove ambiguities in indices and perform `x`- and `tau`-integrals.

```
SimplifyWI[exp_] :=
 SymmetrizeWi@
  SimplifySumQ@
   IntegrateTau@
    Replaceei@IntegrateTrivialTaus@
      Integratex@
       Expand@ApplyDimension@ConvertSumzd@SortQs@exp
```

2.1 Sort Potentials

As a first step in the simplification of the wave invariants we can simplify the arguments of the potentials `Q`.

`SortQs[exp]`
expands the argument of all potentials `Q` in *exp* and sorts the `List` of derivatives.

By Lemma B.4 the arguments of all potentials are transformed into $x + \tau^b l$, where b is some binary multiindex.

```
SortQs[exp_] := exp /. Q[xl_, der_] :> Q[Expand@xl, Sort@der]
```

2.2 Convert Sumzd

The sums over distinct indices of `z` given by `Sumzd` are rather impractical and should be replaced by conventional sums that are expressed using the Einstein convention.

`ConvertSumzd[exp]`
converts all `Sumzd` into conventional sums (still ranging from *1* to *n-1*) given by the Einstein convention.

The idea is to insert a product of all possible factors $(1-\delta_{ij})$ into the sum, where δ_{ij} is the Kronecker delta of some pair of indices of indices, and expand those terms. However, no Kronecker delta will be in the expressions returned. Instead the indices will be transformed and their number reduced according to the Kronecker deltas. Further, not all summands within `Sumzd` contain all indices of this sum. In this case, those indices are removed and a factor of *(n-1)* is added when using the Einstein convention.

Implementation

The Kronecker delta is represented by `Kr[i, j]`, which is thought of as being equal to *1* if the indices given by *i* and *j* are equal and zero otherwise. The definition of the Kronecker delta will not be implemented explicitly.

`Kr[i,j]`
does not evaluate and represents the Kronecker delta δ_{i_i,i_j}.

However, we do not want any Kronecker deltas in our expressions and we just use `Kr` to compute transformation rules that can be applied to the expressions in `Sumzd`. Of course, the transformation rules must be both correct and complete in the sense that all Kronecker deltas are mapped to *1* by the transformations.

Let us start with a `List` of all Kronecker deltas that are needed.

`KrList[indices]`
returns a `List` of all Kronecker deltas of all pairs of *indices*.

```
KrList[indices_] := Kr @@@ Subsets[indices, {2}]
```

We may be tempted to simply form, for example,

```
Expand[Times @@ (1 - KrList[{3, 5, 7}])]
```

```
1 - Kr[3, 5] - Kr[3, 7] + Kr[3, 5] Kr[3, 7] - Kr[5, 7] +
 Kr[3, 5] Kr[5, 7] + Kr[3, 7] Kr[5, 7] - Kr[3, 5] Kr[3, 7] Kr[5, 7]
```

and construct transformation rules from this sum by replacing `Kr` by `Rule`. However, this

does not work for two reasons. Firstly, the term `Kr[3,5]*Kr[3,7]` would give ambiguous transformation rules and secondly the term `Kr[3,5]*Kr[5,7]` would lead to the transformation rules `{3→5,5→7}`. Those two rules are applied concurrently and not sequentially. Thus,

```
f[Wi[3], Wi[5], Wi[7]] * Kr[3, 5] * Kr[5, 7] /. {3 → 5, 5 → 7}
```

```
f[Wi[5], Wi[7], Wi[7]] Kr[5, 7] Kr[7, 7]
```

still contains two indices and one Kronecker delta that may not be omitted.

Hence, we need to change the indices of the Kronecker deltas in such a way that within each summand each index can appear at most once in the left slot of `Kr` and such that any index appearing in the right slot does not appear in any left slot. Assuming that indices within `Kr` are sorted (which they are) this is achieved with the following list of rules provided we apply this list as often as needed.

```
KrRules = {
    Kr[i_, j_] Kr[i_, k_] →
     Kr[i, Max[j, k]] Kr[Min[j, k], Max[j, k]],
    Kr[i_, j_] Kr[j_, k_] → Kr[i, k] Kr[j, k],
    Kr[i_, j_]^_ → Kr[i, j]
   };
```

Those rules do not change the value of the product of the Kronecker deltas involved: The right hand side is 1 for exactly the same values of i, j and k as the left hand side. Thus, those transformation rules are correct. They also assure that unambiguous transformation rules are obtained and that all Kronecker deltas are mapped to 1 upon application of said transformation rules.

Applying `KrRules` greatly reduces the number of summands containing Kronecker deltas. The last rule removes superfluous Kronecker deltas that are sometimes generated by the other two rules.

Now, we could apply `KrRules` to the sum given above and we would obtain correct results. This approach would be rather slow for larger index sets because we would first have to compute a rather large expansion (containing $2^{\text{Number of pairs}}$ summands) and only then apply the simplifying `KrRules`. It is considerably faster to add each factor seperately, expand and apply `KrRules` repeatedly.

`OneMinusKr[indices]`
expands the product of all $(1-\delta_{i_i,i_j})$ for all pairs of *indices* and applies the `KrRules`.

```
OneMinusKr[indices_] :=
 Fold[(#1 - (Expand[#1 * #2] //. KrRules)) &, 1, KrList[indices]]
```

For example,

```
OneMinusKr[{3, 5, 7}]
```

```
1 - Kr[3, 5] - Kr[3, 7] - Kr[5, 7] + 2 Kr[3, 7] Kr[5, 7]
```

Now, those products need to be converted into a `List` containing the transformations given by the Kronecker deltas of a given summand and the corresponding coefficient. This is achieved by substituting `Kr` by `Rule`. (It would have been possible to use `Rule` instead of `Kr` everywhere, at the cost of legibility.)

```
KrToRules[Kr[i1_, i2_]] := {1, Rule[i1, i2]}
KrToRules[summand_] :=
 {summand /. _Kr → 1, Cases[summand, _Kr] /. Kr → Rule}
```

`IndexRules[indices]`
returns a `List` of coefficients and transformation rules that transform a sum `Sumzd` with distinct indices into a conventional sum `sumz`.

An explicit definition is needed when there is only one index.

```
IndexRules[indices_] :=
 IndexRules[indices] =
  KrToRules /@ (List @@ OneMinusKr[indices])
IndexRules[{_}] = {{1, {}}};
```

Finally, we can define `ConvertSumzd`: For every `Sumzd[ind, arg]` we first compute the transformation rules for the given indices *ind*, take the coefficients from this `List` and multiply those with conventional sums `sumz` obtained from each sublist of transformation rules. Here, `sumz[ind, exp]` is a conventional sum over the argument *exp*, where the

indices *ind* each range from *1* to *n-1*.

The transformations are applied to both the index set *ind*, where duplicate indices are removed, and to the argument. In the latter case, we do not want that the transformation rules apply to all integers, but only those that are an argument of `Wi`. Further, the argument is expanded, which is assumed in the evaluation of `sumz` below.

```
ConvertSumzd[exp_] :=
 exp /. Sumzd[ind_, arg_] :> With[{rules = IndexRules@ind},
    Plus @@ (rules[[All, 1]] * Map[
         sumz[
           Union[ind /. #],
           Expand[
            arg /. (# /. Rule[i_, j_] → Rule[Wi[i], Wi[j]])]
          ] &,
         rules[[All, 2]]])]
```

Now, we have replaced the sums over distinct `z`-indices by conventional sums denoted by `sumz` and it is convenient to express those sums with the Einstein summation convention. Not all summation indices in *ind* of `sumz[ind,exp]` must also appear within *exp*. If they do appear they must be an index of `Wi`. Thus, we add a factor *(n-1)* for each index which does not appear as an argument of `Wi`.

Further, it is understood that the Einstein convention for indices of `Wi` represents sums ranging from *1* to *n-1*, while the indices of the `ei` range from *1* to *n*.

```
sumz[indices_, exp_] :=
 exp *
  (n - 1) ^
   (Length@indices -
     Length@Union@Cases[exp, Wi[i_] → i, Infinity])
```

This replacement must be applied to each summand individually.

```
sumz[indices_, exp_Plus] := sumz[indices, #] & /@ exp
```

Example

Consider the following sum with distinct indices:

```
EXs = Sumzd[{3, 5}, f[Wi[3]]];
```

The transformation rules are given by

```
EXr = IndexRules@EXs[[1]]
```

```
{{1, {}}, {-1, {3 → 5}}}
```

with the following coefficients and transformation rules:

```
EXr[[All, 1]]
```

```
{1, -1}
```

```
EXr[[All, 2]]
```

```
{{}, {3 → 5}}
```

Applying those rules to the indices and the argument gives (`sumz` already evaluated)

```
EXev = Map[
  sumz[
    Union[{3, 5} /. #],
    Expand[
     f[Wi[3]] /. (# /. Rule[i_, j_] → Rule[Wi[i], Wi[j]])]
   ] &,
  EXr[[All, 2]]]
```

```
{(-1 + n) f[Wi[3]], f[Wi[5]]}
```

and the multiplication with the coefficients yields

```
EXr[[All, 1]] * EXev
```

```
{(-1 + n) f[Wi[3]], -f[Wi[5]]}
```

Thus, overall the sum with distinct indices is converted into the following combination of two conventional sums.

```
ConvertSumzd[EXs]
```

```
(-1 + n) f[Wi[3]] - f[Wi[5]]
```

Note that we can combine both sums by renaming the indices. This will be done later.

```
Clear[EXs, EXr, EXev]
```

2.3 Apply Dimension

`ApplyDimension[`*exp*`]`
: if a numerical dimension has been specified using `SetDimension[`*dim*`]` then every occurence of `n` is replaced by *dim*.

```
ApplyDimension[exp_] :=
 If[DimensionNQ, exp /. n → dimension, exp]
```

2.4 x-Integral

The `x`-integration must take the factor $E_{-Fl}(x)$ into account, even though we have dropped it from our expressions.

`Integratex[`*exp*`]`
: simplifies some of the expressions in *exp* by considering them as an integrand against the factor $E_{-Fl}(x)$ with respect to `x`. It is assumed that *exp* is in expanded form.

`Integratex` must be linear and it maps all summands that are free of `x` to zero.

```
Integratex[exp_Plus] := Integratex /@ exp
Integratex[exp_?FreexQ] := 0
```

If there is only one potential and its coefficient is free of `x` then the `x`-integral is given by

`QmFl`
: the Fourier coefficient of `Q` with respect to *-Fl*

times a factor for the derivatives. `QmFl` is understood to still depend on `x`, confer Definition 4.46. Although we replace the `AD` by `Ft` later and although `AD[#,l]-`

`AD[l,#]` is the same as `-Ft[l,#]` it is better not to use `Ft` here, for technical reasons.

```
ADXl[Xl_] := Times @@ ((AD[#, l] - AD[l, #]) & /@ Xl)
Integratex[Q[_, der_] * (c : _?FreexQ : 1)] :=
 QmFl * ADXl[der] * c
```

If none of the previous cases apply then we return the expression exp.

```
Integratex[exp_] := exp
```

We have for example:

```
Integratex[Q[x + l tau[2], {}] tau[1]^2 tau[2]^3]
```

```
QmFl tau[1]^2 tau[2]^3
```

```
Integratex[Q[x + l tau[2], {}] Q[x + l tau[1] tau[2], {}] tau[2]]
```

```
Q[x + l tau[2], {}] Q[x + l tau[1] tau[2], {}] tau[2]
```

2.5 Integrate Trivial τ's

The simplification of `Integratex` removes some `tau`'s from the expressions and for this reason we can perform some of the `tau`-integrals at this point. We call a variable `tau[i]` in some summand *trivial* if it does not appear within the arguments of any potential in this summand. For example, in

```
Q[x + tau[2] l, {}] tau[1] tau[2]^2
```

```
Q[x + l tau[2], {}] tau[1] tau[2]^2
```

the variable `tau[1]` is trivial while `tau[2]` is not. All `tau`-variables are integrated from 0 to 1 but only the trivial variables can be integrated (for now).

`IntegrateTrivialTaus[exp]`
integrates all trivial `tau`-variables from 0 to 1.

```
IntegrateTrivialTaus[exp_Plus] := IntegrateTrivialTaus /@ exp
IntegrateTrivialTaus[exp_] := exp /. TrivialTauRules[exp]
```

To compute the tau-integrals we first need find a list of all tau-indices.

```
TauIndices[exp_] :=
 DeleteDuplicates@Cases[exp, tau[i_] → i, {0, Infinity}]
```

The indices of the trivial tau-variables is then the Complement of those tau-variables appearing within a potential within the set of all tau-variables.

```
TrivialTauIndices[exp_] :=
 Complement[TauIndices@exp,
  Flatten@Cases[exp, Q[arg_, _] :> TauIndices@arg,
    {0, Infinity}]]
```

The trivial tau-variables are all of the form τ_i^k and the integration is given by the usual integration rules for polynomials.

```
TrivialTauRules[exp_] :=
 (tau[#]^i_. → 1 / (i + 1)) & /@ TrivialTauIndices[exp]
```

For example,

```
IntegrateTrivialTaus[Q[x + l tau[2], {}] tau[1] tau[2]^2]
```

$$\frac{1}{2}\,\text{Q[x + l tau[2], \{\}] tau[2]}^2$$

We might be tempted to use the standard *Mathematica* function Integrate to compute the trivial tau-integrals. Because this function is very general and cannot use anything known a-priori about the expressions to be integrated, it is much slower.

2.6 Replace e_i

In the construction of the partial wave invariants we have used two orthonormal basis for $\mathbb{R}^n$: The standard basis represented by ei, using even indices, and the Wi, which use odd indices and form an orthonormal basis together with the given normalized lattice vector $l/|l|$. Because the ei originate from the x-derivatives in the x-Laplacian each summand of the partial wave invariants contains each ei[i] in order 2 or not at all. In other words, each summand is a trace with respect to the basis ei and because traces

are independent of the chosen basis we can replace the `ei` basis by the basis `Wi` together with $l/\!\!/l/\!\!/$.

`Replaceei[`*exp*`]`
: replaces in *exp* the basis `ei` in every trace by the basis `Wi` together with `l/nl`. Also, the `Wi`-indices are reduced in the sense that if there are k distinct `Wi`-indices present in some summand then those indices are from the set $\{1,\ldots,k\}$.

The `Wi` do not necessarily appear in order 2 and thus we can only replace the `ei` by `Wi` and $l/\!\!/l/\!\!/$ but not the other way around.

First, `EiList[`*exp*`]` generates a list of all `ei[`i`]` without duplicates and `eitoWiRules[`*eilist*`]` converts this list of `ei[`i`]` into a list of transformation rules. For each `ei[`i`]` we need one summand with `ei[`i`]` replaced by `Wi[`i`]` and one summand with `ei[`i`]` replaced by `l/nl`. `eitoWiRules` generates a list of all tuples from those possibilities.

```
EiList[exp_] := DeleteDuplicates@Cases[exp, _ei, Infinity]

eitoWiRules[eilist_] :=
 eitoWiRules[eilist] =
  Apply[Rule, Transpose[{eilist, #}] & /@
    Tuples@Replace[eilist, eii_ :> {l / nl, Wi @@ eii}, {1}], {2}]
```

For example,

```
eitoWiRules[{ei[1], ei[2]}]
```

$$\left\{\left\{\text{ei}[1]\to\frac{\text{l}}{\text{nl}},\ \text{ei}[2]\to\frac{\text{l}}{\text{nl}}\right\},\ \left\{\text{ei}[1]\to\frac{\text{l}}{\text{nl}},\ \text{ei}[2]\to\text{Wi}[2]\right\},\ \left\{\text{ei}[1]\to\text{Wi}[1],\ \text{ei}[2]\to\frac{\text{l}}{\text{nl}}\right\},\ \{\text{ei}[1]\to\text{Wi}[1],\ \text{ei}[2]\to\text{Wi}[2]\}\right\}$$

We apply each of the tuples of those transformation rules to *exp*, reduce the indices and sum up all resulting expressions.

```
Replaceei[exp_Plus] := Replaceei /@ exp
Replaceei[exp_] :=
 Plus @@ ReduceWi /@ (exp /. eitoWiRules@EiList@exp)
```

To reduce the Wi-indices we need a list of all such indices.

```
WiList[exp_] :=
 DeleteDuplicates@Cases[exp, Wi[i_] → i, Infinity]
```

From this list we can generate a list of rules that maps each index of Wi[i] to its corresponding position in WiList.

```
ReduceWiRules[Wilist_] :=
 Array[(Wi[Wilist[[#]]] → Wi[#]) &, Length@Wilist]
```

Applying those rules to the expression *exp* gives the desired reduction in the Wi-indices.

```
ReduceWi[exp_] := exp /. ReduceWiRules@WiList@exp
ReduceWi[exp_Plus] := ReduceWi /@ exp
```

2.7 Integrate all τ's

The integration of the tau-variables is explained in Chapter B, more specifically Section B.3.

IntegrateTau[*exp*]
: integrates the remaining tau-variables in *exp*. Assumes that *exp* is in expanded form.

The implementation of the integration is split into a section on the collection and structuring of the needed data, two sections on Algorithm I and Algorithm P and a section on the combination thereof. Recall two symbols introduced in Section 0.1.

SumQ[*case*, *exp*]
: is a Q-sum of *exp* over the unintegrated *case*.

Case[c_1, c_2, ...]
: represents the unintegrated cases of varying length.

The formal description of the cases does not use c[*i*] but ct[*i*, l] for technical reasons. This is then corrected at the end of the computation.

Data Gathering

The functions given in this subsection convert the given *summand* into a form that is more suitable to the integration algorithms implemented in the following sections. The first function returns the largest index of any of the `tau`-variables present in the *summand*.

```
Lambda[summand_] :=
 Max[0, Cases[summand, tau[i_] :> i, {0, Infinity}]]
```

Once we know the length of the `tau`-exponent we can extract it.

`TauExponent[exp, lambda]`
returns the multiindex of length *lambda* that is the exponent of `tau` in *exp*.

`TauExponent` requires a seperate definition if *lambda* is greater than zero but the head of *exp* is not `Times`. This can only happen if the expression *exp* is already of the form τ^e with some nonnegative integer e.

```
TauExponent[exp_, lambda_] :=
 ReplacePart[Table[0, {lambda}],
  Cases[exp, tau[i_]^eexp_. :> (i → eexp)]]
TauExponent[tau[i_]^eexp_., lambda_] :=
 ReplacePart[Table[0, {lambda}], i → eexp]
```

The function `TauExponent` can also be used to extract the multiindices b.

`ExtractB[exp, lambda]`
returns the binary multiindices b of length *lambda* contained within *exp*.
The returned multiindices are in flag-form.

By Lemma B.4 all summands are automatically in flag-form, but as was illustrated in Example B.5 in the *Mathematica* canonical order we have to reverse the order of the binary multiindices to achieve flag-form.

```
ExtractB[exp_, lambda_] :=
 Reverse@
  Cases[exp, Q[x + l * taub_, _] :> TauExponent[taub, lambda]]
ExtractB[Q[x + l * taub_, _], lambda_] :=
 {TauExponent[taub, lambda]}
```

After having extracted e and b we want to use both to create the fractured exponent $f(e,b)$. First, we let e denote the `tau`-exponent and B a single binary multiindex.

SelectB[e,B]
returns the submultiindex of e for which the corresponding entries of B are 1.

```
SelectB[e_, B_] := Cases[Transpose@{e, B}, {i_, 1} :> i]
```

For example,

```
SelectB[{1, 2, 3, 4}, {0, 1, 1, 0}]
```

```
{2, 3}
```

Now, with this selection we can fracture e using the multiindices b.

Fracture[e,b]
computes the fractured exponent $f(e,b)$ and sorts its parts.

```
Fracture[e_, b_] :=
 Sort /@
  Fe @@
   (SelectB[e, #] & /@
     Append[Array[(b[[#]] - b[[# + 1]]) &, Length[b] - 1],
      Last@b])
```

Combining the various functions just defined we can extract the fractured exponent of a summand.

ExtractFe[$summand$]
returns the (partially increasing) fractured exponent of the $summand$.

```
ExtractFe[summand_] :=
 Fracture[TauExponent[summand, #], ExtractB[summand, #]] &@
  Lambda@summand
```

Once we have the fractured exponent we can easily obtain the variable partition and an tau-exponent that gives the same integral as the original tau-exponent but is partially sorted.

`VariablePartition[summand]`
returns the variable partition of the *summand*, as determined by its fractured exponent.

`PITauExponent[summand]`
returns the `tau`-exponent of the *summand* as a partially increasing multiindex.

```
VariablePartition[summand_] :=
 List @@ Length /@ ExtractFe@summand
PITauExponent[summand_] := Flatten[List @@ ExtractFe@summand]
```

Example 1

Let us first consider a simple example, the only term with more than one potential appearing in the computation of the second wave invariant.

```
EX = Q[x + l tau[2], {}] Q[x + l tau[1] tau[2], {}] tau[2];
```

The fractured exponent is given by

```
ExtractFe@EX
```

```
Fe[{0}, {1}]
```

and correspondingly the variable partition is

```
VariablePartition@EX
```

```
{1, 1}
```

and the partially increasing `tau`-exponent is given by

```
PITauExponent@EX
```

```
{0, 1}
```

Note that the `Length` of the variable partition is equal to the number of potentials in the summand under consideration and its `Total` is equal to the number of `tau`-variables to

be integrated.

Example 2

Now, let us consider a more complicated example taken from the computation of the fifth wave invariant.

```
EX = Q[x + l tau[3] tau[4] tau[5], {l}]
    Q[x + l tau[1] tau[2] tau[3] tau[4] tau[5], {l}] tau[1]
    tau[3]^2 tau[4]^2 tau[5]^3;
```

Its tau-exponent is not partially increasing:

```
TauExponent[EX, 5]
```

```
{1, 0, 2, 2, 3}
```

However, the fractured exponent is given by

```
ExtractFe@EX
```

```
Fe[{0, 1}, {2, 2, 3}]
```

and thus the partially increasing tau-exponent is

```
PITauExponent@EX
```

```
{0, 1, 2, 2, 3}
```

while the variable partition is

```
VariablePartition@EX
```

```
{2, 3}
```

Example 3

The next example contains only two tau-variables but the largest index is greater than two:

```
EX = Q[x + l tau[3], {}] Q[x + l tau[2] tau[3], {}] tau[2] tau[3]^2;
Lambda@EX
```

```
3
```

Correspondingly, its tau-exponent is longer than needed.

```
TauExponent[EX, Lambda@EX]
```

```
{0, 1, 2}
```

However, this causes no problems as the nonexisting tau-variables are removed during the extraction of the fractured exponent.

```
ExtractFe@EX
```

```
Fe[{1}, {2}]
```

Example 4

While most partially increasing tau-exponents are increasing multiindices some are not. The first such summands appear in the computation of the fourth wave invariant. For example:

```
EX = Q[x + l tau[3] tau[4], {}]
    Q[x + l tau[1] tau[2] tau[3] tau[4], {l}] tau[1] tau[3];
```

Its fractured exponent

```
ExtractFe@EX
```

```
Fe[{0, 1}, {0, 1}]
```

and partially increasing tau-exponent

```
PITauExponent@EX
```

```
{0, 1, 0, 1}
```

are only partially increasing but not increasing.

Finally, we also need the derivatives of the involved potentials. The order of those derivatives has to be reversed because we have reversed the order of the binary multiindices.

`ExtractDer[summand]`
: returns a `List` of the derivatives of the potentials within the *summand* in reversed order.

```
ExtractD[summand_] := Reverse@Cases[summand, Q[_, di_] → di]
ExtractD[Q[_, d1_]] := {d1}
```

Once we have the `List` of derivatives we want to convert this `List` into the expression obtained by applying those derivatives to the Fourier basis elements E_c. Note that the definition of E_c contains a minus sign.

`mctD[d]`
: computes the expression obtained by applying the derivatives d of the potentials to the Fourier basis elements E_c.

See Definition B.2 and Lemma B.6.

```
mctD[d_] := Times @@ (mcti @@@ Transpose@{Range@Length@d, d})
```

Here,

`mcti[i,di]`
: turns the `List` of derivative vectors di of the ith potential into the corresponding `ct`-product.

```
mcti[i_, di_] := Times @@ ((-ct[i, #]) & /@ di)
```

Example

The summand

```
EX = Q[x + l tau[2], {l, Wi[1]}] Q[x + l tau[1] tau[2], {Wi[1]}]
   tau[2];
```

has the derivatives

```
EXd = ExtractD[EX]
```

```
{{Wi[1]}, {1, Wi[1]}}
```

and those contribute the term

```
mctD@EXd
```

```
-ct[1, Wi[1]] ct[2, 1] ct[2, Wi[1]]
```

to the Fourier series of the summand above.

Algorithm I

In this section Algorithm I is implemented.

`AlgorithmI[`*exp*`,`*vph*`]`
applies Algorithm I *vph*-times to *exp*.

As has been mentioned in Section B.3 we need to apply Algorithm I repeatedly and if we are integrating the `tau`-variables belonging to the hth potential then the hth part *vph* of the variable partition gives the number of repetitions needed. Thus, this function integrates all `tau`-variables belonging to the hth potential. If, however, divergent `tau`-coefficients appear then those coefficients stay unchanged for the remaining repetitions of Algorithm I.

Let us start with the trivial integration.

`Intt[`*exp*`]`
integrates the first `tau`-variable in the `tau`-sum or `tau`-coefficient *exp* assuming that the corresponding E-exponent vanishes. Divergent `tau`-coefficients are left unchanged.

`Intt` is linear on sums and removes the first element of the multiindex representing the `tau`-exponent.

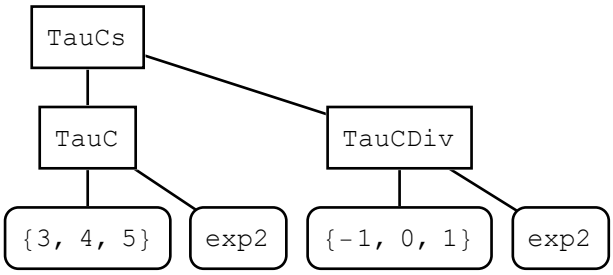
```
Intt[tauCs_TauCs] := Intt /@ tauCs
Intt[tauCDiv_TauCDiv] := tauCDiv
Intt[TauC[e_, exp_]] :=
 CatchDiv@TauC[Rest@e, exp / (1 + e[[1]])]
```

Here, `CatchDiv` is defined below and renames divergent `tau`-coefficients. Even though `Intt` does not return divergent `tau`-coefficients we still need `CatchDiv` here, as negative `tau`-exponents may move to the first position through the removal of the first element of **e**.

Example

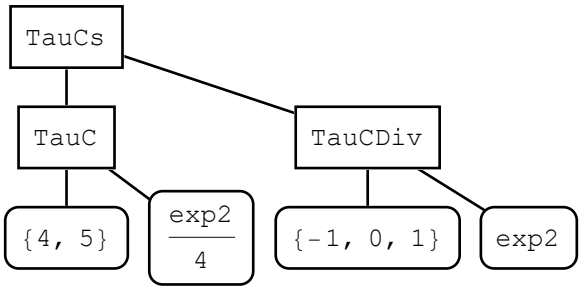
Applying the trivial integration to the following `tau`-sum

```
CTreeForm[
 EX = TauCs[TauC[{3, 4, 5}, exp2], TauCDiv[{-1, 0, 1}, exp2]]]
```



integrates and removes the first `tau`-variable of each nondivergent `tau`-summand and leaves the divergent `tau`-coefficient unchanged:

```
CTreeForm[Intt@EX]
```



The nontrivial integration consists of two functions, `Intp` and `Intm`, that require the E-exponent as an argument. Both are linear on sums and again remove the exponent of

the integrated tau-variable. Their definition is given in Algorithm I in Section B.3.

```
Intp[chl_, tauCs_TauCs] := Intp[chl, #] & /@ tauCs
Intp[chl_, TauC[e_, exp_]] :=
 TauC[Rest[e - (e[[1]] + 1)], e[[1]]! * chl^(-e[[1]] - 1) * exp]
Intm[chl_, tauCs_TauCs] := Intm[chl, #] & /@ tauCs
Intm[chl_, TauC[e_, exp_]] :=
 Sequence @@
  Table[TauC[Rest[e + i - e[[1]] - 1],
    -e[[1]]! / i! * chl^(i - e[[1]] - 1) * exp], {i, 0, e[[1]]}]
```

The treatment of divergent tau-coefficients is slightly more complicated in this case. If Intp and Intm would both return arguments with the head TauCDiv unchanged we would generate superfluous TauCDiv-terms. Thus, we set the following:

```
Intp[_, _TauCDiv] := Sequence[]
Intm[_, tauCDiv_TauCDiv] := tauCDiv
```

Note that Sequence[] splices no argument into the superior Ec and that this corresponds to Intp mapping divergent tau-coefficients to 0.

Now, we can define a single application of Algorithm I.

AlgorithmI[*exp*]
: applies Algorithm I once to exp.

AlgorithmI is linear on sums and distinguishes vanishing and nonvanishing E-exponents. It leaves not only the divergent tau-coefficients unchanged but also preserves their E-coefficients. Intp and Intm may generate multiindices e with $e_1 < 0$, i.e. divergent tau-coefficients. The plus and minus parts of the nontrivial integration are not added but instead we use Sequence in order to splice both expressions into the superordinate ***ecs_Ecs***.

```
AlgorithmI[exp_Plus] := AlgorithmI /@ exp
AlgorithmI[SumQ[case_, ecs_]] :=
 SumQ[case, AlgorithmI /@ ecs]
AlgorithmI[ecs_Ecs] := AlgorithmI /@ ecs
```

```
(* Only needed for the examples. *)
AlgorithmI[Ec[0, tauCs_]] := Ec[0, Intt@tauCs]
AlgorithmI[Ec[chl_, tauCs_]] :=
 Sequence[CatchDiv[Ec[0, Intp[chl, tauCs]]],
  CatchDiv[Ec[chl, Intm[chl, tauCs]]]]
```

The function `CatchDiv` renames the head of all such divergent `tau`-coefficients to `TauCDiv`. Additionally, the expression `Ec[0]` that may appear due to divergent `tau`-coefficients represents an empty sum and is mathematically equal to `0`. It is removed here.

```
CatchDiv[exp_] :=
 exp /. TauC[e_ /; Length@e > 0 && e[[1]] < 0, lexp_] :>
   TauCDiv[e, lexp]
CatchDiv[Ec[0]] := Sequence[]
```

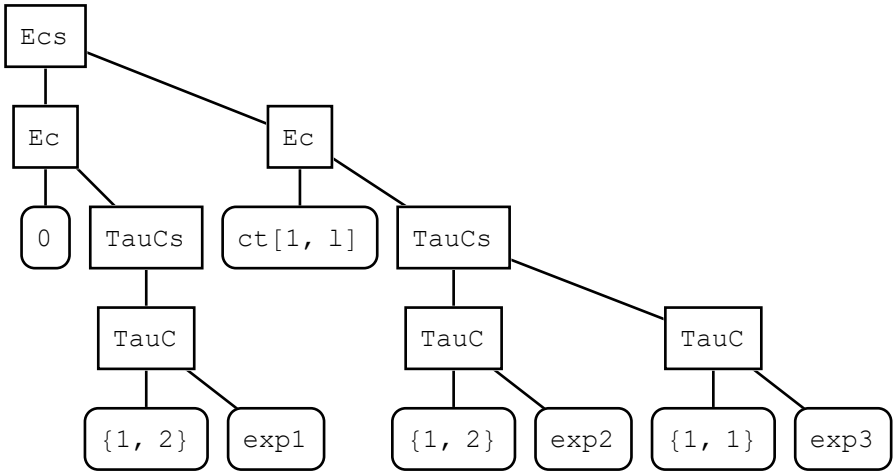
We have set `Intm` to return the divergent `tau`-coefficients because then its E-coefficient is preserved. Applying this function `AlgorithmI` vph-times yields the desired function.

```
AlgorithmI[exp_, vph_] := Nest[AlgorithmI, exp, vph]
```

Example

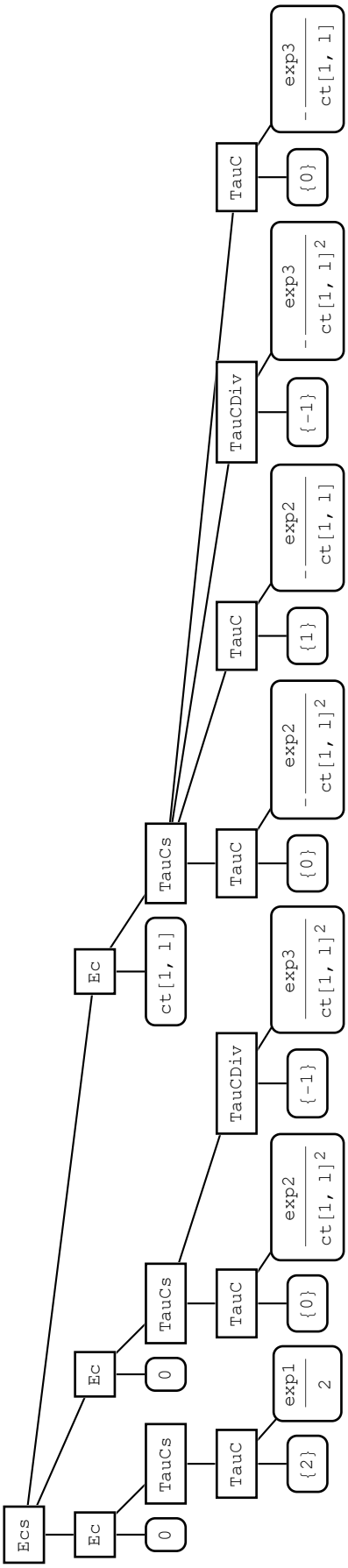
Consider the following expression.

```
CTreeForm[
 EX = Ecs[Ec[0, TauCs[TauC[{1, 2}, exp1]]],
   Ec[ct[1, l], TauCs[TauC[{1, 2}, exp2], TauC[{1, 1}, exp3]]]]]
```



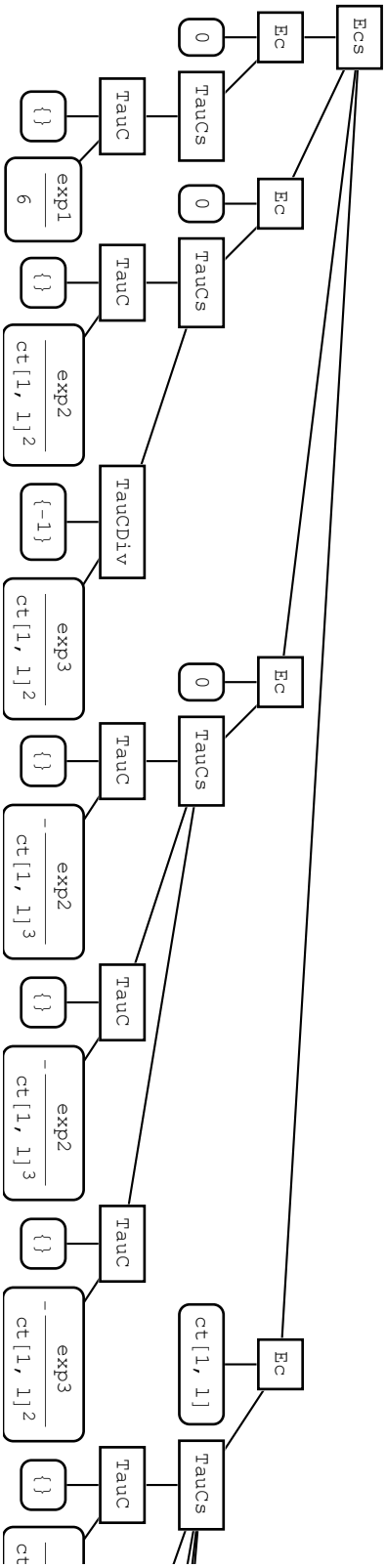
It contains a vanishing and a nonvanishing E-exponents and three `tau`-coefficients with corresponding `tau`-exponents. The trivial integration is applied to the first summand, the nontrivial one to the second summand. Both the trivial and the nontrivial integration return one vanishing E-exponent and those `tau`-exponents that are not strictly increasing lead to divergent `tau`-coefficients:

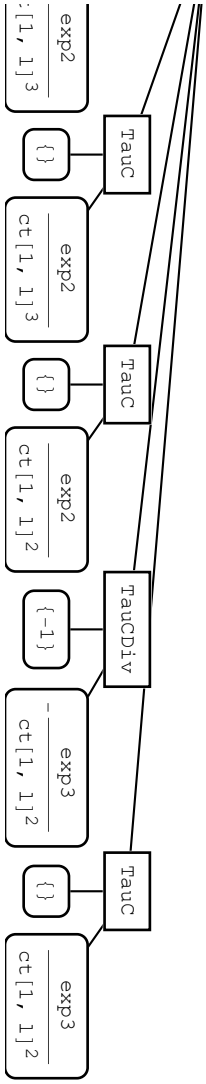
```
CTreeFormR[AlgorithmI@EX]
```


Ecs
Ec
0
TauCs
TauC
{2}
exp1/2
0
Ec
TauCs
TauC
{0}
exp2/ct[1, 1]^2
TauCDiv
{-1}
exp3/ct[1, 1]^2
ct[1, 1]
Ec
TauCs
TauC
{0}
exp2/ct[1, 1]^2
TauC
{1}
exp2/ct[1, 1]
TauCDiv
{-1}
exp3/ct[1, 1]^2
TauC
{0}
exp3/ct[1, 1]

Applying Algorithm I a second time integrates the remaining `tau`-variable but leaves the divergent `tau`-coefficients unchanged.

```
CTreeFormL[AlgorithmI[EX, 2]]
```





It is clear that this expression can be simplified considerably and this shall be done below.

Algorithm P

Let us now implement Algorithm P. We have to generate new cases and apply Algorithm I.

In Definition B.18 we have defined a function `nc` that generates new unintegrated cases given some unintegrated case. Here we define a slightly different function.

`NewCtl` [*case*]
: returns the `List` of `ct`[*h*+*1*,*l*] that must be added to the *case* to obtain the new cases.

```
NewCtl[Case[]] := {0, ct[1, l]}
NewCtl[case_] :=
 Union[(-Plus @@ Take[case, -#]) & /@ Range@Length@case,
  {0, ct[Length@case + 1, l]}]
```

Here, `ct[i,l]` denotes $\tilde{c}_i(l)$ while we have used only the dual lattice vectors c_i in Definition B.18. We could also use the latter here and denote them by `c[i]` but then we would need to perform substitutions `c[i_]→ct[i,l]` within Algorithm P and I. It is simpler to use a slightly longer notation for the unintegrated cases and transform the cases to the desired form upon completion of the `tau`-integration.

Example

```
NewCtl[Case[ct[1, l]]]
```

```
{0, -ct[1, l], ct[2, l]}
```

The list of new cases of `Case[ct[1]]` is thus

```
Append[Case[ct[1, l]], #] & /@ NewCtl[Case[ct[1, l]]]
```

```
{Case[ct[1, l], 0],
 Case[ct[1, l], -ct[1, l]], Case[ct[1, l], ct[2, l]]}
```

The reason for generating a list of the last elements of the formal tuples describing the unintegrated cases is that we need to add $\tilde{c}_{new}(l)$ to every E-exponent, where c_{new} is the last element of the new case.

`NewCases[SumQ[case,ecs]]`
: returns the sum of `SumQ`s over all cases in `nc(case)` and adds $\tilde{c}_{new}(l)$ to every E-exponent in ecs.

```
NewCases[SumQ[case_, ecs_]] :=
 Plus @@
  (SumQ[Append[case, #], EcsTimesEc[ConsolidateEcs@ecs,
       #]] & /@ (NewCtl@case))
```

Before adding $\tilde{c}_{new}(l)$ to the E-exponents we first merge all summands in ecs with equal E-exponents, see Remark B.24.

`ConsolidateEcs[ecs]`
merges those `Ec` in *ecs* that have the same E-exponent.

```
ConsolidateEcs[ecs_] := Ecs @@ Replace[
   Transpose /@ GatherBy[List @@ ecs /. Ec → List, First],
   List[list1_, list2_] :> Ec[First@list1, Join @@ list2],
   {1}]
```

If we add a new dual lattice vector c_{new} to our case we have to add this c_{new} to every E-exponent. This corresponds to a multiplication of *ecs* by $E_{c_{new}}\left(l\tau^{b_{new}}\right)$, where the binary multiindices are already contained in the variable partition.

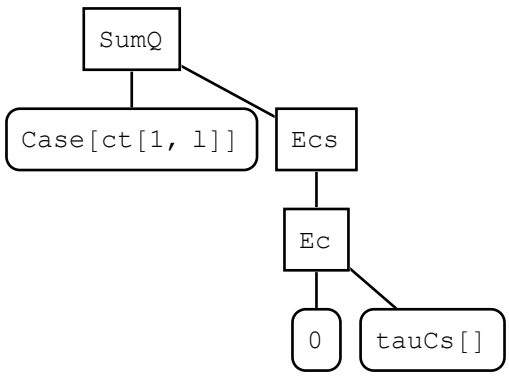
`EcsTimesEc[ecs,ctnewl]`
adds *ctnewl* to every E-exponent in *ecs* and then sorts the obtain expressions by its E-exponents.

```
EcsTimesEc[ecs_, ctnewl_] :=
 SortBy[MapAt[(# + ctnewl) &, ecs, {All, 1}], First]
```

Example

Let us generate new cases for the following expression. Here, `tauCs[]` represents any `tau`-sum.

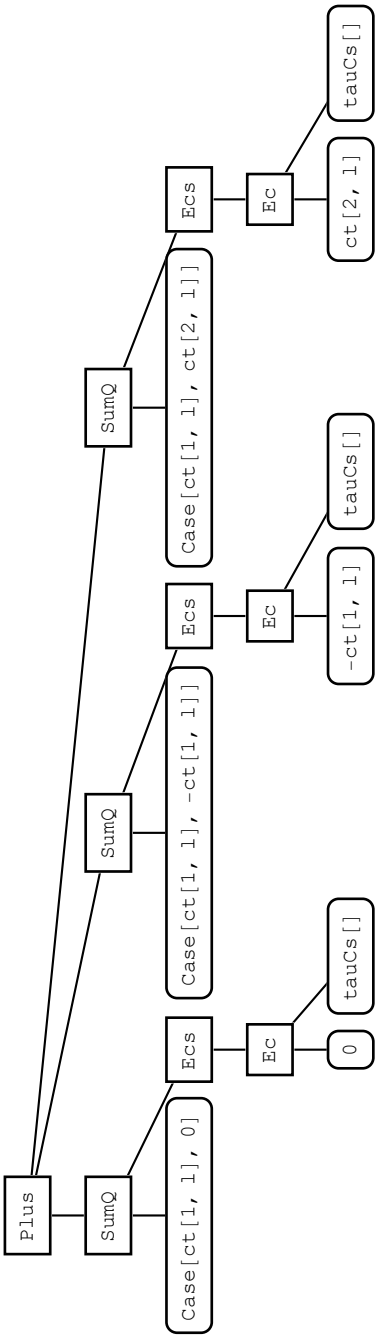
```
CTreeForm[EX = SumQ[Case[ct[1, l]], Ecs[Ec[0, tauCs[]]]]]
```



As we have seen above three new cases are generated and thus we have a sum of three `SumQ`. The new lattice vectors are added to the unintegrated cases and to the E-

exponents.

```
CTreeFormR[NewCases[EX]]
```



We want to apply the function `NewCases` only to sums that do not contain divergent `tau`-coefficients, because such coefficients should stay unchanged. We split our `SumQ` into two such sums, where one contains all divergent `tau`-coefficients represented by `TauCDiv` and the other only nondivergent `tau`-coefficients represented by `TauC`.

SelectDiv[*sumQs*]
: returns the subexpression of *sumQs* that contains only divergent tau-coefficients.

SelectNonDiv[*sumQs*]
: returns the subexpression of *sumQs* that contains only nondivergent tau-coefficients.

```
SelectDiv[sumQs_] :=
 sumQs /. _TauC → Sequence[] /. Ec[_, TauCs[]] → Sequence[] /.
   SumQ[_, Ecs[]] → 0 /. SumQ → SumQDiv
SelectNonDiv[sumQs_] :=
 sumQs /. _TauCDiv → Sequence[] /. Ec[_, TauCs[]] → Sequence[] /.
  SumQ[_, Ecs[]] → 0
```

We start our integration with the InductionBase and then apply Algorithm I and P as dictated by the variable partition.

AlgorithmP[*sumQ*, *vph_Integer*]
: If the second argument *vph* is an Integer then NewCases and AlgorithmI are applied to *sumQ*. After the computation of the integrals the result is split into its divergent and nondivergent parts.

AlgorithmP[*sumQ*, *vph_List*]
: If the second argument is a List and *vp* represents a variable partition then the previous function of AlgorithmP is applied repeatedly with the elements *vph* of *vp* as a second argument.

```
AlgorithmP[a_. * sumQ_SumQ, vph_Integer] :=
 (a SelectDiv@# + a SelectNonDiv@#) &@
  AlgorithmI[NewCases@sumQ, vph]
AlgorithmP[exp_, vp_List] := Fold[AlgorithmP, exp, vp]
```

AlgorithmP is linear in its first argument and leaves expressions with head SumQDiv unchanged.

```
AlgorithmP[a_. * sumQDiv_SumQDiv, vph_Integer] := a * sumQDiv
AlgorithmP[exp_Plus, vph_Integer] := AlgorithmP[#, vph] & /@ exp
```

Combination

With the necessary data we can construct the induction base for the integration algorithm and apply Algorithm I and P.

`InductionBase[e,d]`
: provides the start of the induction of Algorithm P. Contains the partially increasing `tau`-exponent e and the derivatives d but does not contain the information given by the variable partition.

```
InductionBase[e_, d_] :=
 SumQ[Case[], Ecs@Ec[0, TauCs@TauC[e, mctD@d]]]
```

After completing the `tau`-integration we can remove the special heads `Ecs`, `Ec`, `TauCs` and `TauC` that were introduced specifically for the `tau`-integration, at least in the nondivergent case. We can remove `Ec`, because after all `tau`-variables are integrated the exponent within `Ec` is an element of $2\pi i\mathbb{Z}$ and the corresponding exponential is equal to one. Thus, we remove those heads or replace them by conventional heads.

A bit more care is needed in the divergent case: To distinguish divergent `tau`-coefficients with the same `tau`-exponent (after integration) but different fractured exponents we need the variable partition vp and we cannot remove the E-exponents as there are still `tau`-variables present in their exponents.

`ReduceSumQ[exp,vp]`
: removes the special heads in exp, includes the variable partition vp in the divergent `tau`-coefficients and applies `NewCases` to some of the divergent `tau`-coefficients.

After the `tau`-integration is completed there is no need to keep the distinction between `SumQ` and `SumQDiv`. The latter is renamed to `SumQ`.

```
ReduceSumQ[exp_, vp_] := exp /.
      {SumQ[case_, lexp_] :> SumQ[case, lexp /. Ec → (#2 &)],
       sumQDiv_SumQDiv :> ReduceSumQDiv[sumQDiv, vp]} /.
     {Ecs → Plus, TauCs → Plus, TauC → (#2 &)} /. Ec[_, 0] → 0 /.
  SumQ[_, 0] → 0
```

The reformulation of the `SumQDiv`-terms is contained within `ReduceSumQDiv`.

```
ReduceSumQDiv[sumQDiv_, vp_] :=
 NewCasesTauCDiv[
  sumQDiv /. tauCDiv_TauCDiv :> MapAt[CutVP[vp], tauCDiv, {1}]]
```

It is not sufficient to only store the exponents of the unintegrated `tau`-variables but we also need to know between what variables an application of `NewCases` would be necessary. However, storing both the remaining variables and the entire variable partition is unnecessary because it contains those applications of `NewCases` that have already been applied. We reduce the variable partition by removing those variables that have already been integrated.

`CutVP[vp,e]`
: removes those parts of the variable partition vp that have already been integrated and groups the returned variable partition and the `tau`-exponent e into a single object with head `V`.

```
CutVP[vp_][e_] := V[CutVP[{}, vp, Length@e], e]

CutVP[cvp_, vp_, nrtaus_] := If[Last@vp ≤ nrtaus,
  CutVP[Prepend[cvp, Last@vp], Most@vp, nrtaus - Last@vp],
  Prepend[cvp, nrtaus]
 ]
```

Example

The following example stems from a `tau`-integration of a summand with two potentials and four `tau`-variables of which one has been integrated.

```
CutVP[{1, 3}][{-1, 0}]
```

```
V[{2}, {-1, 0}]
```

If, however, we consider the following summand

```
CutVP[{1, 2}][{-1, 0}]
```

```
V[{0, 2}, {-1, 0}]
```

then the zero indicates that the first `tau`-variable in the divergent `tau`-coefficient “belongs” to the next potential and that the corresponding `NewCases` has *not* been

applied during the execution of AlgorithmP.

Regarding those terms that have a reduced variable partition that starts with zero we have two options: We could either leave them as they are or we could apply NewCases once. Both options lead to correct results but the latter has the advantage that it allows divergent tau-coefficients originating from different tau-integrations to cancel. After this modification there is no need to keep the distinction between SumQ and SumQDiv. So we replace the latter by the former.

```
NewCasesTauCDiv[SumQDiv[case_, exp_]] :=
 SumQ[case, exp /. TauCDiv[V[{0, __}, _], _] → 0] +
  NewCases@
   SumQ[case,
    exp /. {TauCDiv[V[cvp_, e_], lexp_] /; cvp[[1]] == 0 :→
       TauCDiv[V[Rest@cvp, e], lexp], _TauCDiv → 0}]
```

Finally, combining everything constructed in this section gives us the desired tau-integration.

IntegrateTau[*exp*]
: integrates the remaining tau-variables in *exp*. Assumes that *exp* is in expanded form.

```
IntegrateTau[exp_Plus] := IntegrateTau /@ exp
IntegrateTau[summand_] :=
 (summand /. {_tau → 1, _Q → 1}) *
    ReduceSumQ[
     AlgorithmP[InductionBase[PITauExponent@summand,
       ExtractD@summand], #], #] &@
  (VariablePartition@summand)
```

If there is no tau-variable present nothing needs to be done.

```
IntegrateTau[summand_ /; FreeQ[summand, _tau]] := summand
```

2.8 Simplification of SumQ

In this section we define a number of simplifications for expressions involving SumQ. We

sort the unintegrated cases, merge sums with equal such cases, use the information contained in the cases and apply an x-integration. All of this will be combined in the following function:

SimplifySumQ[*exp*]
: simplifies expressions involving SumQ in the expression *exp*.

Integration of x

We have already used the x-integration to perform some simplification of summands containing at most one potential Q. Here, we remove all those terms that appear in SumQ with an unintegrated case that cannot be integrated and that do not contain the variable x, see Remark B.22.

ReduceNonzeroCase[*exp*]
: remove the constants from those unintegrated cases that do not add up to zero.

First, we introduce a function that tests whether a given unintegrated *case* does not add up to zero.

```
NonzeroCaseQ[case_] := Not[Plus @@ case === 0]
```

If we have a SumQ with such an unintegrated case then all its summands that are nondivergent and that do not contain the variable x must vanish.

```
ReduceNonzeroCase[exp_] :=
 exp /. SumQ[case_?NonzeroCaseQ, lexp_] :>
   SumQ[case, RemoveConstants@Expand@lexp]
```

RemoveConstants deletes those summands in *lexp*. More summands can be removed if the sum is in expanded form.

```
RemoveConstants[exp_Plus] := DeleteCases[exp, _?FreexdivQ]
RemoveConstants[exp_] := If[FreexdivQ@exp, 0, exp]
```

FreexdivQ tests whether *exp* is free of x and nondivergent. Note that if the option Speed is set via SetSpeed then all *exp* are a priori free of x.

```
FreexdivQ[exp_] := FreexQ[exp] && FreeQ[exp, _TauCDiv]
```

Example

In the computation of the fourth wave invariant the term

```
EX = SumQ[Case[0, ct[2, l]], 39/32 - n/2 + n^2/32];
```

appears. Its case is clearly does not add up to zero

```
NonzeroCaseQ[First@EX]
```

```
True
```

and therefore the summands vanish under `x`-integration.

```
ReduceNonzeroCase@EX
```

```
SumQ[Case[0, ct[2, l]], 0]
```

Sort Case

We can reduce the number of distinct unintegrated cases by renaming `ct[i,l]`-variables such that those that vanish are all at the beginning of the cases.

`SortCase[exp]`
: moves all zeros up front in all cases in *exp*.

To sort the zeros and nonzeros in a case we first need to know their positions. The following functions give a `List` of those indices *i* with *case*`[[i]]` is `0` and the complement of those indices.

```
FindZeros[case_] := Flatten@Position[case, 0, {1}]
FindNonZeros[case_] :=
 Complement[Range@Length@case, FindZeros@case]
```

With `FindZeros` we can test whether the `Case` of some `SumQ` is sorted or not.

CaseSortedQ[*sumQ*]
returns True exactly if all zeros of the case of *sumQ* are at its beginning.

```
CaseSortedQ[sumQ_] :=
 And @@ NonNegative[Range@Length@# - #] &@FindZeros@First@sumQ
```

Now, we apply SortCase to all expressions with head SumQ. But if their case is already sorted then the expression remains unchanged.

```
SortCase[exp_] := exp /. sumQ_SumQ :> SortCase[sumQ]
SortCase[sumQ_SumQ?CaseSortedQ] := sumQ
```

If we have a SumQ with a Case that is not sorted then we seek the first index corresponding to a nonzero entry

```
FirstNonZero[case_] := First@FindNonZeros@case
```

and then the first index that is both larger than this index and that corresponds to a zero entry

```
FirstSwapZero[case_] :=
 First@DeleteCases[FindZeros@case, c_ /; c < FirstNonZero@case]
```

The fact that *case* is not sorted guarantees that the List returned by DeleteCases does indeed have at least one element and thus that First is well-defined. Once we have those two indices, *fnz* and *fsz*, we can rename the indices. Note that it is not sufficient to merely swap the variables ct[*fnz*,l] and ct[*fsz*,l], because the entries in *case* between those two might contain the first nonzero entry. Thus, we move the zero at *fsz* to the position *fnz* of the first nonzero entry and move all entries between *fnz* and *fsz-1* by one position. Of course, we also have to rename the corresponding variables in the summands. The following function provides the needed transformation rules.

```
SortCaseRules[fnz_, fsz_] :=
 {ct[i_ /; fnz ≤ i && i < fsz, v_] -> ct[i + 1, v],
  ct[fsz, v_] → ct[fnz, v]}
```

With those rules we can now change the SumQ.

```
SortCase[SumQ[case_, exp_], fnz_, fsz_] :=
 SumQ[Insert[Delete[case, fsz], 0, fnz], exp] /.
  SortCaseRules[fnz, fsz]
```

After we have moved one out-of-place zero up front we reapply `SortCase` until the *case* is sorted.

```
SortCase[SumQ[case_, exp_]] :=
 SortCase[SortCase[SumQ[case, exp], FirstNonZero@case,
   FirstSwapZero@case]]
```

Examples

The following two summands appear in the computation of the fourth wave invariant:

$$\text{EX} = \text{SumQ}\left[\text{Case}[0, \text{ct}[2, \text{l}]], -\frac{1}{\text{ct}[2, \text{l}]}\right] + \text{SumQ}\left[\text{Case}[\text{ct}[1, \text{l}], 0], \frac{1}{\text{ct}[1, \text{l}]}\right];$$

and if we apply `SortCase` we obtain

```
SortCase[EX]
```

$$\text{SumQ}\left[\text{Case}[0, \text{ct}[2, \text{l}]], -\frac{1}{\text{ct}[2, \text{l}]}\right] + \text{SumQ}\left[\text{Case}[0, \text{ct}[2, \text{l}]], \frac{1}{\text{ct}[2, \text{l}]}\right]$$

The first summand remains unchanged while the `ct`-variables of the second summand are swapped. In particular, those two summands now cancel once we implement the linearity of `SumQ`.

Linearity

In the computation of the wave invariants many expressions with head `SumQ` appear that have the same (unintegrated) case. Those sums can be merged. The same holds for expressions with head `Ec` and `TauCDiv` if their first arguments coincide.

`LinearSumQ[exp]`
implements the linearity of expressions with head `SumQ`, `Ec`, and `TauCDiv` in *exp*.

The linearity of the heads `SumQ`, `Ec` and `TauCDiv` must take the first argument into account and we also want linearity with respect to multiplication by coefficients. The linearity is of the same structure for all three heads and we define one function to implement the linearity for all three heads.

First, we define the linearity with respect to multiplication.

```
LinearTimes[head_][c_. * head_[arg1_, exp_]] :=
 head[arg1, Expand[c * exp]]
LinearTimes[head_][exp_Plus] :=
 LinearTimes[head] /@ CPlus @@ exp
LinearTimes[head_][exp_] := exp
```

The head `CPlus` is introduced here, because pulling in factors might generate equal summands that would then give undesired factors again.

```
LinearPlus[head_][exp_Plus] :=
 With[{explt := LinearTimes[head][exp]},
  Plus @@ (head[#[[1, 1]], Plus @@ Last@#] & /@
       Transpose /@ GatherBy[Cases[explt, _head] /. head → List,
         First]) +
    Plus @@ Cases[explt, Except[_head]]
 ]
LinearPlus[head_][c_. * head_[arg1_, arg2_]] :=
 head[arg1, Expand[c * arg2]]
LinearPlus[_][exp_] := exp
```

Example

Let us first consider an artificial example to clarify the workings of `LinearPlus`.

```
EX = exp0 + f[1, exp1] + f[1, exp2] + f[3, exp3];
```

First, we split the expression into those part with head `f` and those without it. `GatherBy[_, First]` groups the first part by their first arguments.

```
EX2 = GatherBy[Cases[EX, _f] /. f → List, First]
```

```
{{{1, exp1}, {1, exp2}}, {{3, exp3}}}
```

The elements of this list are now transposed. Then, the first list contains the first argument multiple times while the second list contains those expressions that are to be added.

```
Transpose /@ EX2
```

```
{{{1, 1}, {exp1, exp2}}, {{3}, {exp3}}}
```

In the final step, we take the first element of each first list and sum the second lists. As head we resubstitute `f`. Overall:

```
LinearPlus[f][EX]
```

```
exp0 + f[1, exp1 + exp2] + f[3, exp3]
```

Now, we have to apply `LinearPlus` three times for each of the heads we want to be linear. We also remove trivial Q-sums.

```
LinearSumQ[exp_] :=
 LinearPlus[SumQ][Expand@exp] /.
    SumQ[case_, epexp_] :↦ SumQ[case, LinearPlus[Ec][epexp]] /.
  Ec[ct_, ecexp_] :↦ Ec[ct, LinearPlus[TauCDiv][ecexp]] /.
 SumQ[_, 0] → 0
```

We cannot set `TauCDiv[_,0]:=0` or `Ec[_,0]:=0` because this would interfere with the `tau`-integration earlier. The last substitution removes trivial `SumQ`.

Symmetrize ct

Before defining the symmetrization of the `ct`-variables let us motivate this section with an example.

Example

Consider the following summand within SumQ.

```
EX = SumQ[Case[ct[1, l], -ct[1, l]], -1/16 ct[1, l]];
```

Its case states that the sum of the two variables ct[1,l] and ct[2,l] must always be zero. This is of course also true if we swap the indices of the variables and the hidden use of the ct-variables as indices of the Fourier coefficients of Q in SumQ is symmetrical. Therefore, EX is equal to the sum

```
SumQ[Case[ct[1, l], -ct[1, l]], -1/16 ct[2, l]];
```

To this sum we can apply the information contained within its case. EX is equal to

```
SumQ[Case[ct[1, l], -ct[1, l]], 1/16 ct[1, l]];
```

which is only possible if EX vanishes.

There are also summands that do not vanish individually but cancel with other summands under the above substitution.

```
SumQ[Case[ct[1, l], -ct[1, l]],
  -(nl^4 ct[1, Wi[1]]^2 ct[1, Wi[2]]^2)/(960 ct[1, l]) -
   nl^4 ct[2, Wi[1]]^2 ct[2, Wi[2]]^2/(960 ct[1, l])];
```

Instead of trying to find the variable substitution that is needed and check that it is compatible with the given case, we will construct *all* substitutions that are allowed by the case. Each of those substitutions is applied to the second argument of SumQ and the results are summed (and divided by the number of substitutions).

We follow Section B.4.

SymmetrizeCt[*exp*]
symmetrizes the ct-variables in SumQ-expressions within *exp* taking their case into account. It is assumed that the all cases are sorted.

To symmetrize the ct-variables we compute permutations of variables that are acceptable with respect to the case of SumQ. The list of permutations is transformed into a list of substitution rules. Each of those substitutions is applied to *exp* and yields equal (under summation) expressions. Those expressions are summed up and to leave the overall sum unchanged we divide by the number of expressions. Mean does exactly that.

```
SymmetrizeCt[a_. * SumQ[case_, exp_]] :=
 a
  SumQ[case,
   Mean[exp /. PermToRule /@ AcceptablePermutations[case]]]
SymmetrizeCt[exp_Plus] := SymmetrizeCt /@ exp
SymmetrizeCt[exp_] := exp
```

Here, PermToRule transforms a permutation (i.e. a list of integers) into a list consisting of substitution rules.

```
PermToRule[perm_] :=
 MapIndexed[Rule[ct[#1, v_], ct[First@#2, v]] &, perm]
```

For example,

```
PermToRule[{2, 1}]
```

```
{ct[2, v_] → ct[1, v], ct[1, v_] → ct[2, v]}
```

The difficult part is to compute the permutations that are compatible with the case. We first note that all variables that satisfy ct[*i*,1]=0 can be permuted and they can never be permuted with variables that corrspond to nonzero entries in the case. Thus, we split the case into a part consisting of zeros and a (reduced) remainder.

```
AcceptablePermutations[case_] := JoinPermutations @@@ Tuples[
   {Permutations@Range@Length@Cases[case, 0],
    AcceptablePermutations@NonzeroCase@case}
  ]
```

At this point we use that the function SortCase has been applied before the ct-

symmetrization such that all zeros in the *case* are found at the beginning of the case. Further, “reduced” means that we decrease the indices of the `ct`-variables in the nonzero subcase such that they start with `1`.

```
NonzeroCase[case_] :=
 Subcase @@ Cases[case, Except[0]] /.
  ct[i_, l] → ct[i - Count[case, 0], l]
```

For example,

```
NonzeroCase[Case[0, 0, ct[3, l], -ct[3, l]]]
```

```
Subcase[ct[1, l], -ct[1, l]]
```

We give this remainder the head `Subcase` so that the `AcceptablePermuations`-function can recognise those cases that contain no zero entries. Once we have the acceptable permutations of both parts of the case we form all pairs of those permutations using `Tuples` and join those pairs. However, when joining two such pairs we undo the variable shift in the second permutation.

```
JoinPermutations[perm1_, perm2_] :=
 Join[perm1, Length@perm1 + perm2]
```

Let us now generate those lists of formal sums that describe the case under consideration.

`Sums0[`*case*`]`
: returns those formal sums that evaluate to `0` for elements of *case*.

```
Sums0[case_] :=
 IndToEq /@ Select[Subsets[Range@Length@case, {2, Infinity}],
   Sum0Q@case]
```

We consider all subsets of the set of indices and test whether the corresponding formal sum is zero. Sums of length one are automatically nonzero, because we have assumed that every entry of *case* is nonzero.

```
Sum0Q[case_][subset_] := Apply[Plus, case[[subset]]] === 0
```

Here, `IndToEq[indL]` converts a list of indices into the corresponding sum of `ct`-variables.

```
IndToEq[indL_] := Plus @@ (ct[#, l] &) /@ indL
```

On the other hand, to find the list `SumsN0[case]` of never vanishing formal sums we first seek all indices i for which the corresponding entry of the case is `ct[i,l]` and then construct the set of corresponding ends.

```
CtPositions[case_] :=
 Cases[Range@Length@case, i_ /; case[[i]] === ct[i, l]]
SumsN0[case_, i_] := (IndToEq@Range[#, i]) & /@ Range[1, i - 1]
SumsN0[case_] :=
 Flatten[SumsN0[case, #] & /@ (CtPositions@case)]
```

Example

For the unintegrated case

```
EX = Case[ct[1, l], ct[2, l], -ct[2, l]];
```

the vanishing sums are

```
Sums0[EX]
```

```
{ct[2, l] + ct[3, l]}
```

and the never vanishing sums are

```
SumsN0[EX]
```

```
{ct[1, l] + ct[2, l]}
```

The sums consist of summands of the form `ct[i,l]` for technical reasons: The cases have entries of this form and we can reuse the function `CaseToRules` later to again convert cases to substitution rules.

```
CaseToRules[case_] :=
 Rule @@@
  (Transpose@{ct[#, 1] & /@ Range@Length@case, List @@ case} /.
    {exp_, exp_} → Sequence[])
```

Trivial rules are removed in `CaseToRules`.

In the test of permutations for acceptability we want to know whether the formal sums generated from the never vanishing formal sums are subsets of the never vanishing formal sums—up to sign.

`SubsetPMQ[sums1,sums2]`
: returns true if *sums2* without sums of length one is a subset of the union of *sums1* and *-sums1*.

```
SubsetPMQ[sums1_, sums2_] :=
 SubsetQ[Join[sums1, -sums1],
  DeleteCases[sums2, Except[_Plus]]]
```

We are now ready to define a function that tests whether a given permutation is acceptable.

`AcceptablePermutationQ[sums0,sumsN0,caserules][permrules]`
: returns true if the permutation given by its substitution rules *permrules* is acceptable. The case with respect to which this is tested is supplied via its zero and never vanishing formal sums and its substitution rules.

```
AcceptablePermutationQ[sums0_, sumsN0_, caserules_][
  permrules_] :=
 MatchQ[Union[sums0 /. permrules /. caserules], {} | {0}] &&
  SubsetPMQ[sumsN0 /. caserules,
   sumsN0 /. permrules /. caserules]
```

The vanishing formal sums are matched against `{}` as well as `{0}` because there are unintegrated cases, which have no vanishing formal sums. In this case, *sums0* will be empty. Finally, we generate all permutations and select those that are known to be acceptable.

AcceptablePermutations[*case*]
returns a list of acceptable permutations for *case*. It is assumed that all entries in *case* are nonzero.

```
AcceptablePermutations[subcase_Subcase] :=
 Select[Permutations@Range@Length@subcase,
  AcceptablePermutationQ[Sums0@subcase, SumsN0@subcase,
   CaseToRules@subcase]@PermToRule@# &]
```

We did not prove that this function generates all acceptable permutations, only that all returned permutations are indeed acceptable.

Examples

Let us look at the permutations computed to be acceptable. First, if we consider a case with only zero entries then all permutations are acceptable.

```
AcceptablePermutations[Case[0, 0, 0]]
```

```
{{1, 2, 3}, {1, 3, 2}, {2, 1, 3}, {2, 3, 1}, {3, 1, 2}, {3, 2, 1}}
```

On the other hand we can find cases that have no acceptable permutations other than the identity.

```
AcceptablePermutations[Case[ct[1, l], -ct[1, l], ct[3, l]]]
```

```
{{1, 2, 3}}
```

Most of the cases are in between those two extrema. The following Q-sum appears in the fourth wave invariant. Its case admits 8 out of 24 permutations.

```
AcceptablePermutations[
 EX = Case[ct[1, l], -ct[1, l], ct[1, l], -ct[1, l]]]
```

```
{{1, 2, 3, 4}, {1, 4, 3, 2}, {2, 1, 4, 3}, {2, 3, 4, 1},
 {3, 2, 1, 4}, {3, 4, 1, 2}, {4, 1, 2, 3}, {4, 3, 2, 1}}
```

Applying those permutations to its summand yields the following Q-sum.

```
EX = SymmetrizeCt[SumQ[EX, 3/ct[1, l]^3 + 1/(2 ct[1, l]^2)]]
```

```
SumQ[Case[ct[1, l], -ct[1, l], ct[1, l], -ct[1, l]],
 1/8 (6/ct[1, l]^3 + 1/ct[1, l]^2 + 6/ct[2, l]^3 + 1/ct[2, l]^2 +
    6/ct[3, l]^3 + 1/ct[3, l]^2 + 6/ct[4, l]^3 + 1/ct[4, l]^2)]
```

This sum is not simpler but indeed more complicated than the sum we started with. However, in the next section we will define the function `ApplyCase` which uses the information contained in its case. This function reduces this sum.

```
ApplyCase@EX
```

```
SumQ[Case[ct[1, l], -ct[1, l], ct[1, l], -ct[1, l]], 1/(2 ct[1, l]^2)]
```

Applying the Case

The unintegrated *case* in `SumQ[case,exp]` contains information that can be used to simplify the expression *exp*.

`ApplyCase[exp]`
: replaces instances of `ct[i,l]` within expressions with head `SumQ` according to the information contained within their unintegrated case.

```
ApplyCase[a_. * SumQ[case_, exp_]] :=
  a SumQ[case, exp /. CaseToRules@case]
ApplyCase[exp_Plus] := ApplyCase /@ exp
ApplyCase[exp_] := exp
```

The function `CaseToRules` converts the *case* into a list of transformation rules.

Example

In the third wave invariant we have a (divergent) expression

```
EX = SumQ[Case[ct[1, l], -ct[1, l]],
    Ec[0, TauCDiv[V[{1}, {-1}],
      (I nl)/(4 ct[1, l]) + (I nl ct[2, l])/(2 ct[1, l]^2) + (I nl ct[2, l]^2)/(4 ct[1, l]^3)]]];
```

that simplifies to zero when using the information contained within *case*. That is: `ct[2,l]` can be replaced by `-ct[1,l]`.

```
CaseToRules@Case[ct[1, l], -ct[1, l]]
```

```
{ct[2, l] → -ct[1, l]}
```

```
ApplyCase@EX
```

```
SumQ[Case[ct[1, l], -ct[1, l]], Ec[0, TauCDiv[V[{1}, {-1}], 0]]]
```

Combine Simplifications

Finally, we need to combine the simplifications defined in this section into a single simplification function.

`SimplifySumQ[`*exp*`]`
: simplifies expressions involving `SumQ` in the expression *exp*.

We have a certain liberty in which order we want to apply the simplifications. The following order is chosen because it is faster than other orders. However, both `SymmetrizeCt` and `LinearSumQ` require the cases to be sorted. So we apply `SortCase` before we apply `SymmetrizeCt` or `LinearSumQ`. Further, the symmetrization only simplifies the `Q`-sums if `ApplyCase` is applied to its results. So we need to use `ApplyCase` after `SymmetrizeCt`.

Before combining all reductions we introduce one other function, which simplifies the arguments of `TauCDiv` and `SumQ` and removes those expressions that vanish.

```
RemoveZeros[exp_] :=
 exp /. TauCDiv[v_, lexp_] :> TauCDiv[v, Together@lexp] /.
     TauCDiv[_, 0] → 0 /. Ec[_, 0] → 0 /.
   SumQ[case_, lexp_] :> SumQ[case, Together@lexp] /.
  SumQ[_, 0] → 0
```

Example

`Together` removes expressions like the following, appearing when using `SetSpeed[Thorough]`,

```
EX = -nl^2 AD[x, l]/(192 ct[1, l]) - nl^2 AD[x, l]/(96 (-ct[1, l] - ct[2, l])) - nl^2 AD[x, l]/(192 ct[2, l]) -
     nl^2 AD[x, l] ct[1, l]/(192 (-ct[1, l] - ct[2, l]) ct[2, l]) -
     nl^2 AD[x, l] ct[2, l]/(192 ct[1, l] (-ct[1, l] - ct[2, l]));
```

from the wave invariants.

```
Together@EX
```

```
0
```

The advantage of `Together` over `Simplify` is that it is faster and more specific.

Overall we define `SimplifySumQ` to be

```
SimplifySumQ[exp_] :=
 RemoveZeros@
  ApplyCase@
   SymmetrizeCt@LinearSumQ@SortCase@ReduceNonzeroCase@exp
```

All divergent `tau`-coefficients have disappeared at the end of this simplification procedure, at least for the wave invariants 1 to 5. In fact, not all parts of the simplification are needed for this purpose but removing the divergent `tau`-coefficients earlier gives no advantage.

2.9 Symmetrize W_i

Just as the `ct`-variables can be symmetrized it is necessary to symmtrize the `Wi`-variables.

SymmetrizeWi[*exp*]
: symmetrizes and simplifies expressions involving Wi-variables in the expression *exp*.

This symmetrization is easier, because the Wi-variables are not restricted by constraints.

For example, the second partial wave invariant computed using the simplifications defined so far but in the Thorough mode, meaning that terms that contain x or at or that are free of Q are not automatically removed, contains the following terms:

```
EX = -1/24 nl^2 AD[x, Wi[1]] AD[x, Wi[2]]^2 AD[Wi[1], l] +
    1/24 nl^2 AD[x, Wi[1]]^2 AD[x, Wi[2]] AD[Wi[2], l];
```

These terms contain the variable x and the form at, which need to cancel by Lemma 4.37 and Lemma 4.41. It is easy to see that those terms do indeed cancel if we rename the indices of the Wi-variables in one of these terms. However, finding an algorithm that assigns names to Wi-variables in such a way that as many terms as possible cancel or simplify is rather difficult for general terms. It is much simpler to symmetrize all summands with respect to the Wi-variables.

Before we can symmetrize the Wi-indices we first need a list of all such indices.

```
WiIndices[exp_] :=
 DeleteDuplicates@Cases[exp, Wi[i_] → i, Infinity]
```

If we have a list of *indices* and some *permutation* of those indices then PermToWiRule returns the corresponding transformation rules. Trivial rules are removed.

```
PermToWiRule[indices_, permutation_] :=
 Map[Wi@# &,
  Rule @@@ Replace[Transpose@{indices, permutation},
    {i_, i_} → Sequence[], {1}], {2}]
```

`WiPermutations[`*exp*`]`
generates a list of lists of substitution rules corresponding to all permutations of the `Wi`-indices in the expression *exp*.

```
WiPermutations[exp_] := WiPermutations[exp, WiIndices@exp]
WiPermutations[exp_, ind_] :=
 PermToWiRule[ind, #] & /@ Permutations[ind]
```

If the dimension is given by a numerical value and if this value happens to be 2 then there is only one `Wi`-variable, which we call `W`, and there is no need for a symmetrization.

```
SymmetrizeWi[exp_] := If[DimensionNQ && dimension === 2,
  exp /. _Wi → W,
  SymmetrizeWi2@exp
 ]
```

If the dimension is not `2` then we apply the following symmetrization.

```
SymmetrizeWi2[exp_Plus] := SymmetrizeWi2 /@ exp
SymmetrizeWi2[c_. SumQ[case_, exp_]] :=
 SumQ[case, SymmetrizeWi2@Expand[c exp]]
SymmetrizeWi2[exp_] := Expand@Mean[exp /. WiPermutations@exp]
```

If we apply this symmetrization to the example above we have

```
SymmetrizeWi[EX]
```

```
0
```

In particular, the summands, that are free of the potential `Q` or contain `at` or `x`, cancel, as required by the necessary conditions of Section 4.6.

Apart from satisfying those necessary conditions the symmetrization of the `Wi`-variables reduces the size of the wave invariants significantly.

```
SetSpeed[Speed]
ByteCount[EX = SimplifyWI[Plus @@ H /@ HIndices[4]]]
ByteCount[SymmetrizeWi@EX]
```

```
558 128
```

```
265 856
```

3 Definition of the Wave Invariants

In this section we first demonstrate that the first five partial wave invariants are independent of the dimension assumed while computing them. After this we introduce several additional simplifications, which do not work when explicitely computing the wave invariants in lower dimensions. Those simplifications are grouped into a `Finish` function.

`Finish[`*exp*`]`
: simplifies the partial wave invariants in dimension `Large` further.

```
Finish[exp_] :=
 Simplifyn[ReplaceFtl@ApplyCase@CurvatureTraces@exp] /.
   SumQRules /. case_Case :> l @@ (case /. ct[i_, l] → c[i])
```

`WI[`*k*`]`
: computes the kth partial wave invariant $\mathrm{WI}_{k,l}(Q)$ for fixed lattice vector l and potential Q.

The kth partial wave invariant is given by the application of `Finish` to the wave invariant computed in `Large` dimensions using `SimplifyWI`.

```
WI[k_] := Finish@WI[k, Large]
```

`SumQRules` contains some further simplifications. The substitution in the cases removes the `t` (for the "tilde") and `l`, both of which where contained in the (unintegrated) cases for purely technical reasons.

```
SumQRules = {
    SumQ[case : Case[ct[1, l], ___], lexp_] :>
     SumQ[case, FullSimplify@lexp],
    SumQ[case : Case[0 ..], lexp_] :>
     SumQ[case,
      Collect[
       lexp /. Trct[1, 1] →
         TrctSq - Sum[Trct[i, i], {i, 2, Length@case}],
       {nl, _n}, Simplify]]};
```

3.1 Independence of Dimension

As has been mentioned in the definition of the `z`-Laplacian the computation of the `z`-derivatives and therefore of the partial wave invariants changes in lower dimensions. Therefore, the wave invariants have to be computed differently for some dimensions. For the first five wave invariants those dimensions are as follows.

```
SetSpeed[Speed]
{#, NeededDimensions@#} & /@ Range[5] // Column
```

```
{1, {Large}}
{2, {Large}}
{3, {2, Large}}
{4, {2, Large}}
{5, {2, 4, Large}}
```

It turns out that the results are actually independent of the chosen dimension. This is trivial for the first two wave invariants and shall be shown for the third, fourth and fifths below.

For this we define the following:

`WI[`k`,`dim`]`
: computes the kth partial wave invariant in dimension dim. Uses memoization and sets the dimension to dim.

By Lemma B.36 all `SumQ`-terms of order k must vanish unless all elements of its case are zero. Since the cases are sorted, this is the case if the last element of a case is `0`.

```
WI[k_, dim_] := WI[k, dim] = (SetDimension[dim];
    SimplifyWI[Plus @@ H /@ HIndices[k]] /.
     SumQ[case_ /; Length@case == k && Last@case =!= 0, _] → 0)
```

We can compute the third and fourth partial wave invariant in dimension `2` and in larger than two dimensions. We do not want to print the results as those are still rather large.

```
WI[3, 2];
WI[3, Large];
```

The partial wave invariant in dimension `2` is given by the partial wave invariant in `Large` dimensions in the sense that if we replace the dimension `n` by `2` and all occurencies of `Wi[i]` by `W` in the expression for `Large` dimensions then this gives the partial wave invariant for dimension `2`.

```
LinearSumQ[WI[3, 2] - (WI[3, Large] /. {n → 2, _Wi → W})]
```

```
0
```

Recall that `LinearSumQ` implements the linearity of `SumQ`.

The same computation is required for the fourth wave invariant but it takes around five minutes to compute.

```
LinearSumQ[WI[4, 2] - (WI[4, Large] /. {n → 2, _Wi → W})]
```

```
0
```

Fifth Wave Invariant

We need to compute the fifth partial wave invariant in three dimensions: `2`, `4` and `Large` and their comparison can be done analogously.

Warning: The computation of the fifth partial wave invariant takes much longer (around seven hours) and requires much more memory (26 GB) than the fourth. Insufficient memory might delay the computation or crash *Mathematica* or other running programs. For this reason, we load the precomputed results instead.

Compressed Results

The compressed results for the fifth partial wave invariant load automatically upon initilization of this notebook. We only need to uncompress them.

```
WI[5, 2] = Uncompress@CompressedWI[5, 2];
WI[5, 4] = Uncompress@CompressedWI[5, 4];
WI[5, Large] = Uncompress@CompressedWI[5, Large];
```

First, we compare the result for `Large` dimensions with the one for dimension `2`.

```
RemoveZeros@
 LinearSumQ[WI[5, 2] - (WI[5, Large] /. {n → 2, _Wi → W})]
```

```
0
```

Again the formula for the case of `Large` dimensions agrees with the one for dimension `2`. The comparison with the result in dimension `4` is not quite so straight forward, because we cannot simply replace the `Wi` by `W`.

```
ByteCount[LinearSumQ[WI[5, 4] - WI[5, Large] /. n → 4]]
```

```
6 075 000
```

However, the result follows if we replace the Einstein conventions of the `Wi[i]` to explicit sums using `W1`, `W2` and `W3`.

```
ReplaceAllWi[exp_] := Fold[ReplaceWi, exp, Range@4]
ReplaceWi[exp_Plus, i_] := ReplaceWi[#, i] & /@ exp
ReplaceWi[SumQ[case_, exp_], i_] :=
 SumQ[case, ReplaceWi[exp, i]]
ReplaceWi[exp_, i_] := If[
  ContainsQ[exp, Wi[i]],
  (exp /. Wi[i] → W1) + (exp /. Wi[i] → W2) + (exp /. Wi[i] → W3),
  exp
 ]
```

The function `ReplaceAllWi` is specific to dimension `4`. It shows again that the result for the `Large` dimensions agrees with the result for dimension `4`.

```
ReplaceAllWi@LinearSumQ[WI[5, 4] - WI[5, Large] /. n → 4]
```

```
0
```

Thus, it is again sufficient to consider the fifth partial wave invariant only in `Large` dimensions.

3.2 Curvature Traces

After we have seen in the previous section that we only need to consider the formula for the partial wave invariants in `Large` dimensions we end their computation by adding some more simplifications. Those do not work in dimension `2`, so we introduce them here and not earlier.

The second wave invariant, computed using the simplifications defined up to this point, contains the following terms:

```
EX = 1/48 nl^2 QmFl AD[l, Wi[1]]^2 -
     1/24 nl^2 QmFl AD[l, Wi[1]] AD[Wi[1], l] +
     1/48 nl^2 QmFl AD[Wi[1], l]^2;
```

Those are equal to

```
Factor@EX
```

$$\frac{1}{48}\,\mathrm{nl}^2\,\mathrm{QmFl}\,(\mathrm{AD}[\mathrm{l},\,\mathrm{Wi}[1]]-\mathrm{AD}[\mathrm{Wi}[1],\,\mathrm{l}])^2$$

and we can replace the occurencies of `AD` by `Ft`. Also, we can replace the sums over the `Wi` by curvature traces.

`CurvatureTraces[`*exp*`]`
: replaces sums over `Wi`-variables in `AD`-expressions in *exp* by traces of the curvature.

As a first step we replace occurencies of `AD` by curvature terms. The first argument of `Ft`

denotes the rank of the curvature trace.

```
ReplaceAD[exp_] :=
 Expand[
  exp /. {AD[y_, l] → Ft[1, l, y] + AD[l, y],
     AD[Wi[i_], Wi[j_]] /; i > j →
      Ft[1, Wi[j], Wi[i]] + AD[Wi[j], Wi[i]]} /.
   SumQ[case_, lexp_] :↦ SumQ[case, Expand@lexp]]
```

Substitutions in one summand lead to cancellations with other summands. To avoid substitutions that undo each other we only substitute `AD` if the second argument is the lattice vector `l` or if both arguments are an `Wi` and their indices are sorted. In the example, we have:

```
ReplaceAD@EX
```

$$\frac{1}{48}\,\text{nl}^2\,\text{QmFl}\,\text{Ft}[1,\text{l},\text{Wi}[1]]^2$$

After having replaced the `AD` by expressions of `Ft` we want to transform sums over the `Wi` into traces. However, there are two things to take into consideration. First, it is (from looking at the formula of the wave invariants so far) not clear that all `Wi` appear in quadratic order and second the `Wi` form an orthonormal base only together with the normalized lattice vector `l/nl`.

To tackle the first problem we introduce a function that counts the order of a given `Wi[j]` within a summand. Note that the wave invariants are fully expanded by `ReplaceAD`.

```
CountWiOrder[Wi[i_], j_] := If[i == j, 1, 0]
CountWiOrder[exp_Times, i_] :=
 Plus @@ (CountWiOrder[#, i] & /@ List @@ exp)
CountWiOrder[Ft[_, x_, y_], i_] :=
 CountWiOrder[x, i] + CountWiOrder[y, i]
CountWiOrder[exp_^p_, i_] := p * CountWiOrder[exp, i]
CountWiOrder[ct[_, x_], i_] := CountWiOrder[x, i]
CountWiOrder[AD[x_, y_], i_] :=
 CountWiOrder[x, i] + CountWiOrder[y, i]
CountWiOrder[at[x_], i_] := CountWiOrder[x]
```

If there were expressions that are neither of the form treated above nor free of `Wi`, i.e.

divergent tau-coefficients, then an error message would be printed,

```
CountWiOrder[exp_, i_] := If[
  FreeQ[exp, Wi[i]],
  0,
  Message[WiTraces::WiOrder, i, exp]; NoWiOrder
 ]
WiTraces::WiOrder =
  "Cannot evaluate the Wi[`1`]-order of `2`.";
```

With this counting function we can define a function that returns a list of all orders in which all Wi-variables appear within a summand.

```
WiOrders[exp_] := CountWiOrder[exp, #] & /@ WiIndices@exp
```

Now, we only proceed if all Wi-variables appear in quadratic order or not at all.

```
WiTracesQ[exp_] := MatchQ[DeleteDuplicates@WiOrders@exp,
  {} | {2}]
```

WiTraces[*exp*]
: is a linear function that replaces sums over Wi-variables *exp* by traces.

```
WiTraces[exp_Plus] := WiTraces /@ exp
WiTraces[SumQ[case_, exp_]] := SumQ[case, WiTraces@exp]
WiTraces[exp_] := If[
  WiTracesQ@exp,
  MakeTr[exp],
  Message[WiTraces::NonWiTraces, exp]; exp
 ]
```

If there were a Wi-variable that is not of quadratic order then an error message would be printed and the expression is returned unchanged.

```
WiTraces::NonWiTraces =
  "There is an Wi[j] that is not of order 2 in `1`.";
```

Note that we first replace all `Ft` by a curvature trace of rank 1 and then the function `MakeTr` transforms the sums over the `Wi` by traces, taking the missing `l/nl` into account.

```
MakeTr[c_. * Ft[i1_, X_, Wi[k_]] * Ft[i2_, Wi[k_], Y_]] :=
 MakeTr[c * Ft[i1 + i2, X, Y] - c * Ft[i1, X, l] Ft[i2, l, Y] / nl^2]

MakeTr[c_. * Ft[k_, Wi[i_], Wi[i_]]] :=
 MakeTr[c * Ft[k] - c * Ft[k, l, l] / nl^2]
```

We apply `MakeTr` repeatedly until all `Wi`-variables have disappeared. If a `Wi`-variable appears as an argument of some `ct` then we pull the `ct` (with index) into the curvature trace or we form a trace over the `ct` only.

```
MakeTr[c_. * ct[i_, Wi[j_]] Ft[k_, Wi[j_], X_]] :=
 MakeTr[c * Ft[k, ct[i], X] - c * ct[i, l] * Ft[k, l, X] / nl^2]
MakeTr[c_. * ct[i_, Wi[j_]] Ft[k_, X_, Wi[j_]]] :=
 MakeTr[c * Ft[k, X, ct[i]] - c * ct[i, l] * Ft[k, X, l] / nl^2]
MakeTr[c_. * ct[i_, Wi[k_]] ct[j_, Wi[k_]]] :=
 MakeTr[c * Sort@Trct[i, j] - c * ct[i, l] ct[j, l] / nl^2]
MakeTr[c_. * ct[i_, Wi[j_]]^2] :=
 MakeTr[c * Trct[i, i] - c * ct[i, l]^2 / nl^2]
```

If the form of our expression is not of the form seen above we use the (anti)commutativity of the curvature traces to reshuffle the arguments so that we can apply the transformations above.

```
MakeTr[c_. * Ft[i_, X_, Wi[k_]]^2] :=
 MakeTr[c Ft[i, X, Wi[k]] * (-1)^i Ft[i, Wi[k], X]]
MakeTr[c_. * Ft[i_, Wi[k_], Y_]^2] :=
 MakeTr[c Ft[i, Y, Wi[k]] * (-1)^i Ft[i, Wi[k], Y]]
MakeTr[c_. * Ft[i1_, X1_, Wi[k_]] Ft[i2_, X2_, Wi[k_]]] :=
 MakeTr[c Ft[i1, X1, Wi[k]] * (-1)^i2 Ft[i2, Wi[k], X2]]
MakeTr[c_. * Ft[i1_, Wi[k_], Y1_] Ft[i2_, Wi[k_], Y2_]] :=
 MakeTr[c Ft[i1, Wi[k], Y1] * (-1)^i2 Ft[i2, Y2, Wi[k]]]
```

Finally, we want `MakeTr` to be linear and to end once all `Wi`-variables have disappeared.

```
MakeTr[exp_Plus] := MakeTr /@ exp
MakeTr[exp_ /; FreeQ[exp, _Wi]] :=
 exp /.
  {Ft[k_, ct[i_], ct[j_]] /; i > j → (-1)^k Ft[k, ct[j], ct[i]],
   Ft[_?OddQ, X_, X_] → 0}
MakeTr[exp_] := exp
```

Once the construction of the traces has ended we close this algorithm by sorting some `ct`-variables and by removing curvature traces that are known to vanish by their anticommutativity. We set

```
CurvatureTraces[exp_] := WiTraces@ReplaceAD@exp
```

Examples

The second partial wave invariant in `Large` dimensions has the form

```
SetSpeed[Speed]
WI[2, Large]
```

$$\frac{15\,\text{QmFl}}{16} - \frac{n\,\text{QmFl}}{2} + \frac{n^2\,\text{QmFl}}{16} + \frac{1}{48}\,\text{nl}^2\,\text{QmFl}\,\text{AD}[l, \text{Wi}[1]]^2 - \frac{1}{24}\,\text{nl}^2\,\text{QmFl}\,\text{AD}[l, \text{Wi}[1]]\,\text{AD}[\text{Wi}[1], l] + \frac{1}{48}\,\text{nl}^2\,\text{QmFl}\,\text{AD}[\text{Wi}[1], l]^2 + \text{SumQ}\left[\text{Case}[0, 0], -\frac{\text{nl}^2}{8}\right]$$

and if convert `Wi`-sums into curvature traces we obtain

```
CurvatureTraces@WI[2, Large]
```

$$\frac{15\,\text{QmFl}}{16} - \frac{n\,\text{QmFl}}{2} + \frac{n^2\,\text{QmFl}}{16} - \frac{1}{48}\,\text{nl}^2\,\text{QmFl}\,\text{Ft}[2, l, l] + \text{SumQ}\left[\text{Case}[0, 0], -\frac{\text{nl}^2}{8}\right]$$

The size of the third partial wave invariant decreases significantly.

```
ByteCount@WI[3, Large]
ByteCount@CurvatureTraces@WI[3, Large]
```

```
20 264
```

```
8800
```

The same holds for the fourth wave invariant.

```
ByteCount@WI[4, Large]
ByteCount@CurvatureTraces@WI[4, Large]
```

```
266 088
```

```
71 624
```

The construction of the curvature traces creates terms that might vanish under a given case. For example, in the third partial wave invariant we have the summands

```
EX = SumQ[Case[0, 0],
    -1/96 ⅈ nl ct[1, l]^2 - 1/96 ⅈ nl ct[1, l] ct[2, l] -
     1/96 ⅈ nl ct[2, l]^2];
```

that vanish when `ApplyCase` is used.

```
ApplyCase@EX
```

```
SumQ[Case[0, 0], 0]
```

3.3 Curvature Traces 2

If a summand in a `SumQ` is free of `x`, which all summands are, then the sum over the `ct[`i`]` must equal `-Ft[l]`. Thus we can replace some curvature terms by sums over `ct[`i`]`.

`ReplaceFtl[`exp`]`
: replaces some curvature terms in exp by sums over `ct[`i`]`-variables.

This function should be linear and the identity on terms not containing `SumQ`.

```
ReplaceFtl[exp_Plus] := ReplaceFtl /@ exp
ReplaceFtl[exp_] := exp
ReplaceFtl[SumQ[case_, exp_]] :=
 SumQ[case, ReplaceFtl[exp, Length@case]]
```

Within the SumQ we replace parts of the curvature traces by sums over ct-variables. The transformations below can create unsorted or vanishing traces. We sort and remove those, respectively.

```
ReplaceFtl[exp_Plus, caselength_] :=
 ReplaceFtl[#, caselength] & /@ exp
ReplaceFtl[exp_?FreexQ, caselength_] := Expand[
  exp /. Ft[i_, l, X_] :>
       -Sum[Ft[i - 1, ct[j], X], {j, 1, caselength}]
     /. Ft[i_, X_, l] :> Sum[Ft[i - 1, X, ct[j]],
       {j, 1, caselength}]
    /. Ft[0, ct[i_], ct[j_]] :> Sort@Trct[i, j]
   /. {Ft[k_?OddQ, X_, X_] → 0,
    Ft[k_, ct[i_], ct[j_]] /; i > j → (-1)^k Ft[k, ct[j], ct[i]]}
 ]
ReplaceFtl[exp_, _] := exp
```

This simplification has no effect on the first two wave invariants. In the third wave invariant it simplifies the following terms.

```
ReplaceFtl@
 SumQ[Case[0, 0], 1/96 i nl^3 Trct[1, 1] + 1/96 i nl^3 Trct[1, 2] +
   1/96 i nl^3 Trct[2, 2] + 1/96 i nl^3 Ft[1, l, ct[1]] +
   1/96 i nl^3 Ft[1, l, ct[2]] - 1/192 i nl^3 Ft[2, l, l]]
SumQ[Case[0, 0], 1/192 i nl^3 Trct[1, 1] + 1/192 i nl^3 Trct[2, 2]]
```

3.4 Simplify n

The wave invariants contain coefficients that depend on the dimension n that can be

simplified. For example, the third partial wave invariant contains

$$\text{EX} = \text{QmFl}\left(-\frac{105\,i}{256} + \frac{11\,i\,n}{16} - \frac{43\,i\,n^2}{128} + \frac{i\,n^3}{16} - \frac{i\,n^4}{256}\right)\Big/\,\text{nl};$$

and the bracket is equal to `-n[1,7] I/256`, see Lemma D.1. The aim of this section is to express those coefficients using `n[i,j]`.

`Simplifyn[exp]`
: expresses coefficients in *exp* using the function `n[i,j]`.

First, we split *exp* into the part of the partial wave invariant that contains `QmFl` and the part that contains `SumQ`. In both parts, we write the sums as polynomials in the (formal) variables `QmFl`, `nl`, `Ft`, `Trct` and `ct` and apply `Formnij`. For the sums in `SumQ` we first form a single rational expression and then apply this `Collectnij` only to the numerator.

```
Collectnij[exp_] :=
 Collect[exp, {QmFl, nl, _Ft, _Trct, _ct}, Formnij]

Simplifyn[exp_] := exp
Simplifyn[exp_Plus] :=
 Collectnij@Select[exp, ContainsQ[#, QmFl] &] +
  Plus @@
   Cases[exp, SumQ[case_, lexp_] :>
     SumQ[case, Collectnij[Numerator@#] / Denominator[#] &@
       Together@lexp]] + Select[exp, FreeQ[#, QmFl | _SumQ] &]
```

We also have a third summand in `Simplifyn` that contains neither `QmFl` nor `SumQ`. In a correct computation of the wave invariants this term must vanish. It is merely added for robustness.

`Formnij[exp]`
: simplifies the coefficient *exp* by introducing the function `n[i,j]`.

If the coefficient does not contain the dimension `n` then nothing needs to be done.

```
Formnij[exp_ /; FreeQ[exp, n]] := exp
```

If the expression *exp* does contain the dimension we form products `n[i,j]` by applying Lemma D.1. We do not assume that *exp* can be expressed using (a single) `n[i,j]`. We

use the highest exponent of n and the second coefficient (after normalization) to compute one n[i,j]. Then we substract this product from *exp* and reapply Formnij to the remainder.

In order to substract n[i,j] from *exp* we need an evaluation of this product.

```
neval[i_, j_] := Product[n - k, {k, i, j, 2}]
```

To apply Lemma D.1 we need the maximal exponent k of n in *exp*, the coefficient C_k of this maximal exponent (to normalize) and the coefficient C_{k-1} of n^{k-1}. The second highest coefficient of the normalized polynomial is then C_{k-1}/C_k. It is not clear that $C_{k-1}/(k \cdot C_k)$ is an integer, so we test whether it is and if not the expression is not changed. This does not occur in the first five wave invariants, though.

```
Formnij[exp_] := Block[{
    k = Exponent[exp, n],
    Ck := Coefficient[exp, n, k],
    Ckm1 := Coefficient[exp, n, k - 1],
    c},
   If[k == 0, exp,
    c = Ckm1 / (k Ck);
    If[
     Not@IntegerQ@c,
     exp,
     (Formnij@Expand[exp - Ck neval@##] + Ck * n@##) &[
      -c - k + 1, -c + k - 1]
    ]
   ]
  ]
```

In the example given above we have

```
Formnij@EX
```

$$-\frac{i\,\text{QmFl}\,n[1,\,7]}{256\,nl}$$

4 Results

This section contains the final results of the computation of the wave invariants. We

briefly repeat the notation introduced in Section 0.1 but only those parts still needed for the results.

`n`
: is any even and positive integer that represents the dimension of the flat torus M under consideration here.

`n[i,j]`
: represents the $n_{i,j} = \prod_{h=0}^{(j-i)/2} n-(i+2h)$ defined in Section D.1.

`l`
: is some fixed nonzero lattice vector in $\mathbb{R}^n$.

`nl`
: denotes the norm of the lattice vector `l`.

Further, we need the curvature form originating from the given connection. Recall, that a tilde over any symbol abbreviates a factor $2\pi i$ and this tilde is represented here by adding the letter `t` to the letter symbolising the mathematical object.

`Ft[X,Y]`
: denotes the curvature $F(X, Y)$ of the connection times the factor $2\pi i$.

`Ft[k,X,Y]` and `Ft[k]`
: are curvature traces defined in Definition 3.7 times the factor $(2\pi i)^k$.

The wave invariants are expressed as functions of the Fourier coefficients of the potential `Q`. Two types of Fourier coefficients appear:

`QmFl`
: is the Fourier coefficient Q_{-Fl} of Q with the index $-F(l)$.

`SumQ[case,exp]`
: is a Q-sum of exp over the integrated or unintegrated $case$.

`l[c1, c2, ...]`
: denotes the (integrated) cases of varying length.

The elements of the cases are denoted similarly to `at`.

`ct[i,Y]`
: represents the ith component $\tilde{c}_i(Y) = 2\pi i c_i(Y)$ of an element of a case applied to the vector Y.

`ctl[alpha]`
: does not evaluate and denotes $\tilde{c}_1(l)^{\alpha_1} \cdots \tilde{c}_k(l)^{\alpha_k}$, where k is the length of the sequence $alpha$.

There are two types of traces over such dual lattice vectors that appear in the wave invariants.

`Trct[i,j]`
denotes the trace over $\tilde{c}_i \cdot \tilde{c}_j$ as a bilinear function.

`TrctSq`
denotes the sum $\tilde{c}_1 \tilde{c}_1 + \cdots + \tilde{c}_k \tilde{c}_k$, where k is the length of the case of the Q-sum that contains this `TrctSq`.

4.1 Wave Invariants

The partial wave invariants can be computed with the function

`WI[k]`
computes the kth partial wave invariant $\mathrm{WI}_{k,l}(Q)$ for fixed lattice vector l and potential Q.

The following computations are all done with the `Speed` setting.

```
SetSpeed[Speed]
```

The first partial wave invariant is very simple.

```
WI[1]
```

$$\frac{\mathrm{i}\ \mathrm{nl}\ \mathrm{QmFl}}{2}$$

The second, third and fourth partial wave invariants are given by the following expression.

```
WI[2]
```

$$\mathrm{QmFl}\left(-\frac{1}{48}\,\mathrm{nl}^2\,\mathrm{Ft}[2,\,1,\,1] + \frac{1}{16}\,\mathrm{n}[3,\,5]\right) + \mathrm{SumQ}\left[\mathrm{l}[0,\,0],\,-\frac{\mathrm{nl}^2}{8}\right]$$

WI[3]

$$\text{QmFl}\left(\text{nl}^3\left(\frac{1}{96}\,\text{i}\,\text{Ft}[2]-\frac{\text{i}\,\text{Ft}[2,\,1,\,1]^2}{2304}\right)-\frac{\text{i}\,\text{n}[1,\,7]}{256\,\text{nl}}+\frac{1}{384}\,\text{i}\,\text{nl}\,\text{Ft}[2,\,1,\,1]\,\text{n}[5,\,7]\right)+\text{SumQ}\left[\text{l}[0,\,0],\,\frac{1}{192}\,\text{i}\,\text{nl}^3\,\text{TrctSq}+\frac{1}{64}\,\text{i}\,\text{nl}\,\text{n}[5,\,7]\right]+\text{SumQ}\left[\text{l}[\text{c}[1],\,-\text{c}[1]],\,-\frac{\text{i}\,\text{nl}^3\,\text{Trct}[1,\,2]}{8\,\text{ct}[1,\,1]^2}\right]+\text{SumQ}\left[\text{l}[0,\,0,\,0],\,-\frac{\text{i}\,\text{nl}^3}{48}\right]$$

WI[4]

$$\text{QmFl}\left(\text{nl}^4\left(-\frac{\text{Ft}[2]\,\text{Ft}[2,\,1,\,1]}{2304}+\frac{\text{Ft}[2,\,1,\,1]^3}{165\,888}-\frac{\text{Ft}[4,\,1,\,1]}{2880}\right)-\frac{\text{n}[-1,\,9]}{6144\,\text{nl}^2}+\frac{\text{Ft}[2,\,1,\,1]\,\text{n}[3,\,9]}{6144}+\text{nl}^2\left(\frac{1}{768}\,\text{Ft}[2]\,\text{n}[7,\,9]-\frac{\text{Ft}[2,\,1,\,1]^2\,\text{n}[7,\,9]}{18\,432}\right)\right)+\text{SumQ}\left[\text{l}[0,\,0],\,\frac{\text{n}[3,\,9]}{1024}+\frac{\text{nl}^2\,\text{TrctSq}\,\text{n}[7,\,9]}{1536}+\frac{\text{nl}^4\left(5\,\text{TrctSq}^2+4\left(-30\,\text{Ft}[2]+\text{Trct}[1,\,2]^2\right)\right)}{46\,080}\right]+\text{SumQ}\left[\text{l}[\text{c}[1],\,-\text{c}[1]],\,-\frac{1}{192\,\text{ct}[1,\,1]^4}\right.\text{nl}^2\left(-24\,\text{nl}^2\,\text{ct}[1,\,1]\,\text{Ft}[1,\,\text{ct}[1],\,\text{ct}[2]]+72\,\text{nl}^2\,\text{Trct}[1,\,2]^2+\text{ct}[1,\,1]^2\,\text{Trct}[1,\,2]\left(3\,\text{n}[7,\,9]+\text{nl}^2\,(\text{Trct}[1,\,1]+2\,\text{Trct}[1,\,2]+\text{Trct}[2,\,2])\right)\right)\left.\right]+\text{SumQ}\left[\text{l}[0,\,0,\,0],\,-\frac{\text{nl}^4\,\text{TrctSq}}{1152}-\frac{1}{384}\,\text{nl}^2\,\text{n}[7,\,9]\right]+\text{SumQ}\left[\text{l}[0,\,\text{c}[2],\,-\text{c}[2]],\,\frac{\text{nl}^4\,\text{Trct}[2,\,3]}{16\,\text{ct}[2,\,1]^2}\right]+\text{SumQ}\left[\text{l}[0,\,0,\,0,\,0],\,\frac{\text{nl}^4}{384}\right]$$

The fifth partial wave invariant is both very large and takes a lot of time and memory to compute. For this reason, the fifth partial wave invariant will be computed in a separate section.

4.2 Small Wave Invariants

From the partial wave invariants we can construct “small” partial wave invariants that are similar but somewhat simpler than the original wave invariants. To obtain them we form

linear combinations of lower order wave invariants. The coefficients of those linear combinations may not depend on the lattice vectors `l` but only on its norm `nl`, confer Theorem 5.8.

```
wi[1] = WI[1] 2 / (I nl)
```

```
QmFl
```

```
wi[2] = LinearSumQ[- (WI[2] - wi[1] n[3, 5] / 16) 8 / nl^2]
```

$$\frac{1}{6}\,\text{QmFl}\,\text{Ft}[2,\,\text{l},\,\text{l}] + \text{SumQ}[\text{l}[0,\,0],\,1]$$

```
wi[3] =
 LinearSumQ[
  (WI[3] / I - wi[2] nl n[5, 7] / 64 +
     wi[1] (n[1, 7] / (256 nl) - Ft[2] nl^3 / 96)) (-48) / nl^3]
```

$$\frac{1}{48}\,\text{QmFl}\,\text{Ft}[2,\,\text{l},\,\text{l}]^2 + \text{SumQ}\left[\text{l}[0,\,0],\,-\frac{\text{TrctSq}}{4}\right] + \text{SumQ}\left[\text{l}[\text{c}[1],\,-\text{c}[1]],\,\frac{6\,\text{Trct}[1,\,2]}{\text{ct}[1,\,\text{l}]^2}\right] + \text{SumQ}[\text{l}[0,\,0,\,0],\,1]$$

```
wi[4] =
 LinearSumQ[
  (WI[4] + wi[3] nl^2 n[7, 9] / 384 +
     wi[2] (-n[3, 9] / 1024 + 120 nl^4 Ft[2] / 46 080) +
     wi[1] (n[-1, 9] / (6144 nl^2) - nl^2 Ft[2] n[7, 9] / 768))
   384 / nl^4]
```

$$\frac{1}{432}\,\text{QmFl}\,\text{Ft}[2,\,\text{l},\,\text{l}]^3 - \frac{2}{15}\,\text{QmFl}\,\text{Ft}[4,\,\text{l},\,\text{l}] + \text{SumQ}\left[\text{l}[0,\,0],\,\frac{\text{TrctSq}^2}{24} + \frac{1}{30}\,\text{Trct}[1,\,2]^2\right] + \text{SumQ}\left[\text{l}[\text{c}[1],\,-\text{c}[1]],\,\frac{48\,\text{Ft}[1,\,\text{ct}[1],\,\text{ct}[2]]}{\text{ct}[1,\,\text{l}]^3} - \frac{2\,\text{Trct}[1,\,1]\,\text{Trct}[1,\,2]}{\text{ct}[1,\,\text{l}]^2} - \frac{144\,\text{Trct}[1,\,2]^2}{\text{ct}[1,\,\text{l}]^4} - \frac{4\,\text{Trct}[1,\,2]^2}{\text{ct}[1,\,\text{l}]^2} - \frac{2\,\text{Trct}[1,\,2]\,\text{Trct}[2,\,2]}{\text{ct}[1,\,\text{l}]^2}\right] + \text{SumQ}\left[\text{l}[0,\,0,\,0],\,-\frac{\text{TrctSq}}{3}\right] + \text{SumQ}\left[\text{l}[0,\,\text{c}[2],\,-\text{c}[2]],\,\frac{24\,\text{Trct}[2,\,3]}{\text{ct}[2,\,\text{l}]^2}\right] + \text{SumQ}[\text{l}[0,\,0,\,0,\,0],\,1]$$

4.3 The Fifth Wave Invariant

In this section we compute the fifth partial wave invariant. It takes several hours and approximately 25 GB of memory to compute. So we load the precomputed result here.

```
WI[5, Large] = Uncompress@CompressedWI[5, Large];
```

The fifth partial wave invariant is rather large

```
ByteCount[WI[5]]
```

```
61 288
```

but is contained in the following subsection.

Fifth Partial Wave Invariant

The corresponding small partial wave invariant is smaller but still relatively large.

Warning: Note that the small partial wave invariants `wi[1]` to `wi[4]` of the previous section need to be computed before one can compute the following fifth small partial wave invariant.

```
wi[5] =
  LinearSumQ[WI[5] 3840 / (I nl^5) + 5 n[9, 11] / (4 nl^2) wi[4] +
      (5 Ft[2] / 3 - 5 n[5, 11] / (8 nl^4)) wi[3] +
     wi[2] (5 n[1, 11] / (32 nl^6) - 5 Ft[2] n[9, 11] / (4 nl^2)) +
     wi[1] (-5 Ft[2]^2 / 12 - Ft[4] / 3 - 5 n[-3, 11] / (256 nl^8) +
        5 Ft[2] n[5, 11] / (16 nl^4))] /.
   SumQ[case_, exp_] :> SumQ[case, Simplify@exp];
ByteCount[wi[5]]
```

```
49 424
```

To reduce the size of this expression we will apply yet another simplification tailored to the fifth partial wave invariant.

`Simplifywi5[exp]`
: is a function defined to simplify the fifth small partial wave invariant.

This function introduces the following multiindex notation:

ctl [*alpha*]
does not evaluate and denotes $\tilde{c}_1(l)^{\alpha_1} \cdots \tilde{c}_k(l)^{\alpha_k}$, where k is the length of the sequence *alpha*.

Result

Simplifywi5@wi@5

```
5 QmFl Ft[2, l, l]^4 / 20736 - 1/18 QmFl Ft[2, l, l] Ft[4, l, l] + SumQ[l[0, 0],
  (-35 TrctSq^3 + 4032 Ft[2, ct[1], ct[1]] - 84 TrctSq Trct[1, 2]^2 - 16 Trct[1, 2]^3)/6048]
 + SumQ[l[c[1], -c[1]], 1/(6 ct[1, l]^6)
  5 (-5760 ct[1, l] Ft[1, ct[1], ct[2]] Trct[1, 2] + 8640 Trct[1, 2]^3 -
     48 ct[1, l]^3 Ft[1, ct[1], ct[2]] (Trct[1, 1] + 3 Trct[1, 2]) + 144 ct[1, l]^2
      (4 Ft[2, ct[1], ct[2]] + Trct[1, 2]^2 (Trct[1, 1] + 2 Trct[1, 2])) +
     ct[1, l]^4 Trct[1, 2] (Trct[1, 1]^2 + 2 Trct[1, 2]^2 +
        Trct[1, 1] (4 Trct[1, 2] + Trct[2, 2])))] +
 SumQ[l[0, 0, 0], 5 TrctSq^2/72 + 1/6 Trct[1, 2]^2] +
 SumQ[
  l[0, c[2], -c[2]],
  -1/ct[2, l]^4 10
   (-24 ct[2, l] Ft[1, ct[2], ct[3]] - 24 Trct[1, 2] Trct[1, 3] + 72 Trct[2, 3]^2 +
     ct[2, l]^2 Trct[2, 3] (Trct[1, 1] + 2 (Trct[2, 2] + Trct[2, 3])))] +
 SumQ[l[c[1], c[2], -c[1] - c[2]], (160 Trct[1, 3]
    (ct[1, l]^2 Trct[1, 2] + ct[2, l] (ct[1, l] + ct[2, l]) Trct[2, 3]))/
   (ct[1, l]^2 ct[2, l]^2 (ct[1, l] + ct[2, l])^2)] +
 SumQ[l[0, 0, 0, 0], -5 TrctSq/12] +
 SumQ[
  l[0, 0, c[3], -c[3]],
  60 Trct[3, 4]/ct[3, l]^2] +
 SumQ[l[c[1], -c[1], c[1], -c[1]],
  -1/(nl^2 ct[1, l]^4) 5 (ct[1, l]^2 (3 n[9, 11] + 4 nl^2 (Trct[1, 1] + Trct[1, 2])) +
     48 nl^2 (4 Trct[1, 2] + Trct[1, 3]))] +
 SumQ[l[c[1], -c[1], c[3], -c[3]], -1/(nl^2 ct[1, l]^3 ct[3, l]^3)
   5 (24 nl^2 ct[1, l] ct[3, l] (2 Trct[1, 2] + Trct[1, 4]) +
     24 nl^2 ct[3, l]^2 (6 Trct[1, 2] + Trct[1, 3] + Trct[1, 4]) +
```

```
      ct[1, l]^2 (ct[3, l]^2 (3 n[9, 11] + 4 nl^2 (Trct[1, 1] + Trct[1, 2])) + 24 nl^2
          (Trct[1, 3] + Trct[1, 4]))))] + SumQ[l[c[1], c[2], -c[2], -c[1]],
    (120 (ct[1, l]^4 (Trct[1, 2] + Trct[1, 3]) + ct[2, l]^4 (Trct[1, 2] + Trct[1, 3]) +
        ct[1, l] ct[2, l]^3 (Trct[1, 2] + 2 Trct[1, 3]) +
        ct[1, l]^3 ct[2, l] (Trct[1, 2] + 2 (Trct[1, 3] + Trct[1, 4])))) /
     (ct[1, l]^3 ct[2, l]^3 (ct[1, l] + ct[2, l])^2)] +
  SumQ[l[c[1], c[2], c[3], -c[1] - c[2] - c[3]],
   (60 (-2 ctl[6, 1, 1, 0] (11 Trct[1, 2] + 10 Trct[2, 3] + 14 Trct[2, 4]) +
        ctl[5, 3, 0, 0] (8 Trct[1, 2] + 8 Trct[1, 3] - 32 Trct[1, 4] +
          6 Trct[2, 3] - 48 Trct[2, 4] - 40 Trct[3, 4]) +
        ctl[6, 2, 0, 0] (-12 Trct[1, 2] - 6 Trct[1, 3] - 30 Trct[1, 4] -
          5 Trct[2, 3] - 42 Trct[2, 4] - 25 Trct[3, 4]) +
        ctl[4, 4, 0, 0] (6 Trct[1, 2] + 66 Trct[1, 3] + 28 Trct[1, 4] -
          33 Trct[2, 3] - 78 Trct[2, 4] - 17 Trct[3, 4]) +
        ctl[5, 2, 1, 0] (34 Trct[1, 2] - 8 Trct[1, 3] - 28 Trct[1, 4] +
          42 Trct[2, 3] + 32 Trct[2, 4] - 14 Trct[3, 4]) +
        2 ctl[4, 3, 1, 0] (29 Trct[1, 2] + 28 Trct[1, 3] + 8 Trct[1, 4] +
          17 Trct[2, 3] + 8 Trct[2, 4] - Trct[3, 4]) - 2 ctl[7, 1, 0, 0]
         (7 Trct[1, 2] + Trct[1, 4] + 6 Trct[2, 3] + 10 Trct[2, 4] + Trct[3, 4]) +
        4 ctl[3, 3, 2, 0] (5 Trct[1, 2] + 20 Trct[1, 3] + 9 Trct[1, 4] +
          Trct[2, 3] - 6 Trct[2, 4] + 6 Trct[3, 4]) +
        ctl[4, 2, 2, 0] (50 Trct[1, 2] - 2 Trct[1, 3] - 2 Trct[1, 4] +
          57 Trct[2, 3] + 78 Trct[2, 4] + 9 Trct[3, 4]))) /
     ((ct[1, l] + ct[2, l])^2 (ct[2, l] + ct[3, l])^2 (ct[1, l] + ct[2, l] + ct[3, l])^2
       ctl[2, 2, 2, 0])] + SumQ[l[0, 0, 0, 0, 0], 1]
```

Implementation

The idea behind this simplification is to "antisymmetrize" the arguments of the Q-sums using acceptable permutations. This does not work well for the 13th and largest summand of the fifth partial wave invariant, which will get a seperate treatment.

```
Simplifywi5[exp_Plus] := Simplifywi5 /@ exp
Simplifywi5[
  SumQ[case : l[c[1], c[2], c[3], -c[1] - c[2] - c[3]], exp_]] :=
 SumQ[case, Simplifywi513@exp]
Simplifywi5[sumQ_SumQ] := AntiSymmetrize@sumQ
Simplifywi5[exp_] := exp
```

The idea of the antisymmetrization is to apply all acceptable permutations to each summand in a Q-sum and then pick those permuted summands that have the lowest `IndexScore`.

`IndexScore[exp]`
: condenses the distribution of `ct`-indices in the expression *exp* into a natural number.

The choice of `IndexScore` and the decision to minimize with respect to this function are somewhat arbitrary.

```
IndexScore[_Plus] := 0
IndexScore[exp_Times] := Plus @@ IndexScore /@ List @@ exp
IndexScore[ct[i_, _]^k_.] := i * Abs@k
IndexScore[Ft[_, ct[i_], ct[j_]]] := i + j
IndexScore[Trct[ct[i_], ct[j_]]] := i + j
IndexScore[nl^_.] := 0
IndexScore[_?NumberQ] := 0
IndexScore[exp_^k_] := Abs[k] * IndexScore@exp
```

Before we can minimize with respect to the `IndexScore` we must (again) define the effect of a permutation on expressions. We will apply permutations to the `ct`-indices of Q-sums but we cannot use function `PermToRule`, because the resulting transformation rules would ignore the notation introduced to reduce the size of the partial wave invariants (`ct[i]`, `ctl[alpha]` and `Trct[i,j]`). Therefore, we introduce a second function turning permutations into transformation rules.

`PermToRule2[perm]`
: computes a list of transformation rules corresponding to the permutation perm that permutes not only the indices of expressions of the form `ct[i,v]` but also `ct[i]`, `ctl[alpha]` and `Trct[i,j]`.

```
PermToRule2[perm_] :=
 {cls_ctl :> Permute[cls, perm], ct[i_] :> ct[perm[[i]]],
  ct[i_, v_] :> ct[perm[[i]], v],
  Trct[i_, j_] :> Trct[perm[[i]], perm[[j]]]}
```

Now, we can define the antisymmetrization.

`Antisymmetrize[SumQ[case,exp]]`
: antisymmetrizes *exp* by minimizing each summand of *exp* with respect to `IndexScore` under permutations acceptable with respect to *case*.

```
AntiSymmetrize[SumQ[case_, exp_]] := SumQ[case, FullSimplify[
   AntiSymmetrize[
     PermToRule2 /@ AcceptablePermutations[
       case /. c[i_] → ct[i, l]],
     CaseToRules[case /. c[i_] → ct[i, l]],
     Expand@exp] /. {Trct[i_, j_] :↦ Trct[Min[i, j], Max[i, j]],
     Ft[k_, ct[i_], ct[j_]] /; i > j :↦
      (-1)^k Ft[k, ct[j], ct[i]]}
  ]
 ]
AntiSymmetrize[exp_] := exp
```

To generate transformation rules we first need to reshape the case to fit the requirements fo `AcceptablePermutations`. We then use `PermToRule2` to obtain transformation rules.

```
AntiSymmetrize[rules1_, rules2_, exp_Plus] :=
 AntiSymmetrize[rules1, rules2, #] & /@ exp
AntiSymmetrize[rules1_, rules2_, summand_] :=
 First@MinimalBy[summand /. rules1 /. rules2, IndexScore]
```

This concludes the definition of the antisymmetrization. Let us continue by defining the special simplification for the 13th summand of the fifth partial wave invariant. This Q-sum has the case

```
First[wi[5][[13]]]
```

```
l[c[1], c[2], c[3], -c[1] - c[2] - c[3]]
```

and thus the acceptable permutations are

```
AcceptablePermutations[First[wi[5][[13]]] /. c[i_] → ct[i, l]]
```

```
{{1, 2, 3, 4}, {1, 4, 3, 2}, {2, 1, 4, 3}, {2, 3, 4, 1},
 {3, 2, 1, 4}, {3, 4, 1, 2}, {4, 1, 2, 3}, {4, 3, 2, 1}}
```

But we only need two of those permutations:

`{2,1,4,3}` and `{3,2,1,4}`.

Further, the expression of this Q-sum is a rational function with the denominator

```
den = Denominator@Last[wi[5][[13]]]
```

```
ct[1, l]^2 ct[2, l]^2 (ct[1, l] + ct[2, l])^2 ct[3, l]^2
 (ct[2, l] + ct[3, l])^2 (ct[1, l] + ct[2, l] + ct[3, l])^2
```

which is the product of the squares of all sums of `ct[i,l]` that are nonvanishing in the given case. It can be checked easily that this denominator remains unchanged under the above two permutations.

```
den /. PermToRule2[{3, 2, 1, 4}]
```

```
ct[1, l]^2 ct[2, l]^2 (ct[1, l] + ct[2, l])^2 ct[3, l]^2
 (ct[2, l] + ct[3, l])^2 (ct[1, l] + ct[2, l] + ct[3, l])^2
```

```
den /. PermToRule2[{2, 1, 4, 3}]
```

```
ct[1, l]^2 ct[2, l]^2 (ct[1, l] + ct[2, l])^2 ct[4, l]^2
 (ct[1, l] + ct[4, l])^2 (ct[1, l] + ct[2, l] + ct[4, l])^2
```

For the latter permutation we have to replace `ct[4,l]` by `-ct[1,l]-ct[2,l]-ct[3,l]` to see that the denominator remains unchanged.

The summands of the numerator on the other hand consists (in expanded form) of a product of `ct[i,l]` and a single `ct`-trace. For example, up to a factor of `60`, the first four summands are:

```
Take[Expand[Numerator@Last[wi[5][[13]]] / 60], 4]
```

```
-2 ct[1, l]^5 ct[2, l] ct[3, l]^2 Trct[1, 2] -
 7 ct[1, l]^4 ct[2, l]^2 ct[3, l]^2 Trct[1, 2] -
 8 ct[1, l]^3 ct[2, l]^3 ct[3, l]^2 Trct[1, 2] -
 2 ct[1, l]^2 ct[2, l]^4 ct[3, l]^2 Trct[1, 2]
```

We first replace the products of `ct[i,l]` by the multiindex notation `ctl[alpha]`. The following function only works for cases of length four. The length of alpha is four, even though the last index is always zero, as the numerator is free of `ct[4,l]`.

```
CtToMultiindex4[exp_Plus] := CtToMultiindex4 /@ exp
CtToMultiindex4[exp_] := CtToMultiindex4[1, ctl[] * exp]
CtToMultiindex4[i_, exp_] := CtToMultiindex4[i + 1,
  If[FreeQ[exp, ct[i, l]],
   exp /. ctMI_ctl :> Append[ctMI, 0],
   exp /. ctMI_ctl * ct[i, l]^k_. :> Append[ctMI, k]
  ]
 ]
CtToMultiindex4[5, exp_] := exp
```

For example,

```
CtToMultiindex4@Take[Expand[Numerator@Last[wi[5][[13]]] / 60],
  4]
```

```
-2 ctl[2, 4, 2, 0] Trct[1, 2] - 8 ctl[3, 3, 2, 0] Trct[1, 2] -
 7 ctl[4, 2, 2, 0] Trct[1, 2] - 2 ctl[5, 1, 2, 0] Trct[1, 2]
```

In order to simplify the numerator we will now apply the two permutations above in order to change the multiindices into multiindices that are decreasing. Note that we can apply the permutations to the numerator because they are acceptable and leave the denominator unchanged.

```
SimplifyNumerator[exp_Plus] := SimplifyNumerator /@ exp
SimplifyNumerator[exp : ctl[i_, j_, k_, 0] * _ /; i ≥ j && j ≥ k] :=
 exp
SimplifyNumerator[exp : ctl[i_, j_, k_, 0] * _ /;
   (i ≥ k && j ≥ i + k) || (i ≥ k && k > j)] :=
 SimplifyNumerator[exp /. PermToRule2[{2, 1, 4, 3}]]
SimplifyNumerator[exp : ctl[i_, _, k_, 0] * _ /; k > i] :=
 SimplifyNumerator[exp /. PermToRule2[{3, 2, 1, 4}]]
```

Those permutations replace the zero-exponents of `ct[4,l]` by some nonzero integer. Those factors are removed by using the information contained in the case and replacing `ct[4,l]` by `-ct[1,l]-ct[2,l]-ct[3,l]`.

```
SimplifyNumerator[exp : ctl[__, Except[0]] * _] :=
 SimplifyNumerator@ctl4@exp
```

The function ctl4 implements this substitution.

```
ctl4[exp_] :=
 Expand[
      exp /. ctl[is__, i4_] →
        ctl[is, 0] * (-ct[1, l] - ct[2, l] - ct[3, l])^i4] /.
    ctl[i1_, is__] * ct[1, l]^k_. → ctl[i1 + k, is] /.
   ctl[i1_, i2_, i3_, i4_] * ct[2, l]^k_. →
    ctl[i1, i2 + k, i3, i4] /.
  ctl[i1_, i2_, i3_, i4_] * ct[3, l]^k_. → ctl[i1, i2, i3 + k, i4]
```

Finally, we have to combine all the above function into the single function Simplifywi513.

```
Simplifywi513[exp_] :=
 60
  Collect[
    SimplifyNumerator@CtToMultiindex4@
       Expand[Numerator@exp / 60] /.
     Trct[i_, j_] /; i > j → Trct[j, i], _ctl, Simplify] /
   CtToMultiindex4@Denominator@exp
```

5 Miscellaneous

5.1 Relation to Heat Invariants

Although the wave invariants are not defined for the case *l=0* we can nevertheless evaluate the small wave invariants in this case. Using the heat invariants we can show that the wave invariants are still spectral invariants in this case.

Warning: The small wave invariants must have been computed and the initialization cells of the notebook computing the heat invariants must have been executed for the following to run.

To compare the higher small wave invariants with the heat invariants we first remove those terms that vanish if the lattice vector l is zero. Also, we express TrctSq as an explicit sum of traces and replace SumQ by SumQ0. In the latter we will implement

simplifications. All cases must be of the form `l[0,...,0]` and it is thus sufficient to remember the length of each case.

```
wil0[k_] :=
 wi[k] /. {Ft[_, _, l] → 0, SumQ[case_ /; Last@case =!= 0, _] → 0,
   SumQ[case_, exp_] :→
    SumQ0[Length@case,
     Expand[exp /. TrctSq → Sum[Trct[i, i], {i, Length@case}]]]}
```

We want `SumQ0` to undo the effect of the Fourier expansion. First, it should be linear.

```
SumQ0[case_, exp_Plus] := SumQ0[case, #] & /@ exp
SumQ0[case_, c_Rational * exp_] := c * SumQ0[case, exp]
```

Apart from this, `SumQ0` should replace traces `Trct` be the corresponding derivatives of the potential `Q`. This alone would not show equality with the heat invariants. We also need to apply `IntegrationByParts` of the notebook of the heat invariants to compute some simplifications. Hence, we need to use the form `Q[0,der]` of the potential used in this notebook.

```
SumQ0[case_, 1] := Q[0, {}]^case
SumQ0[case_, Trct[i_, i_]^k_.] := Q[0, {}]^(case - 1) Q[k, {}]
SumQ0[case_, Trct[i_, i_]^k_. Trct[j_, j_]^h_.] :=
 Q[0, {}]^(case - 2) Q[k, {}] Q[h, {}]

SumQ0[case_, Trct[i_, j_]^k_.] :=
 Q[0, {}]^(case - 2) Q[0, ei /@ Range@k]^2
SumQ0[case_, Ft[k_, ct[i_], ct[i_]]] :=
 Q[0, {}]^(case - 1) Ft[k, ei[1], ei[2]] Q[{ei[1], ei[2]}]
SumQ0[case_, (Trct[i_, j_] | Trct[j_, i_])^k_. *
   Trct[j_, j_]^h_.] :=
 Q[0, {}]^(case - 2) Q[0, ei /@ Range@k] Q[h, ei /@ Range@k]
```

For example, we have

```
SumQ0[2, Trct[1, 1]^2 Trct[2, 2]]
```

```
Q[1, {}] Q[2, {}]
```

Combining those definitions we have for the third small wave invariant that for *l=0*

```
wil0[3]
```

$$Q^3 - \frac{1}{2} Q\, Q[1]$$

and for the heat invariants that

```
Expand[-6 HeatInvariant[6] - Ft[2] HeatInvariant[2] / 2]
```

$$Q^3 - \frac{1}{2} Q\, Q[1]$$

Both are equal, as claimed. For the fourths small wave invariant we have

```
wil0[4] - Expand[24 HeatInvariant[8] + 2 Ft[2] HeatInvariant[4]]
```

$$\frac{Ft[2]^2}{12} - \frac{Ft[4]}{15} - \frac{7}{60} Q\, Q[2] + \frac{1}{30} Q[0, \{ei[1], ei[2]\}]^2 + \frac{1}{12} Q[1, \{\}]^2$$

but `IntegrationByParts` shows equality up to a constant.

```
IntegrationByParts@wil0[4] -
 Expand[24 HeatInvariant[8] + 2 Ft[2] HeatInvariant[4]]
```

$$\frac{Ft[2]^2}{12} - \frac{Ft[4]}{15}$$

The same holds for the fifths small wave invariant:

```
IntegrationByParts@wil0[5] -
 Expand[-HeatInvariant[10] 120 - 10 Ft[2] HeatInvariant[6] -
   (5 / 12 Ft[2]^2 - Ft[4] / 3) HeatInvariant[2]]
```

```
0
```

This shows that the first five small wave invariants for *l=0* are given by the heat invariants and are indeed spectral invariants, as well.

5.2 Lemma 6.12

The more tedious calculations of the proof of Lemma 6.12 is automated here. First we compute the supported parts of the cases appearing in the partial wave invariants. The set of dual lattice vectors that do not vanish when applied to lattice vector `l` are

```
nz = {Fl1, -Fl2};
```

and the vectors in `-nz`. The sign in `nz` is chosen such that both elements are equal when applied to `l`. We now look for all tuples of these dual lattice vectors that also satisfy the conditions of the case in question.

```
ValidTuples[sets_] :=
 Select[Tuples@sets, Plus @@ # == -Fl1 - Fl2 &]
GenerateTuples[sets_] :=
 Join[ValidTuples[sets], ValidTuples[-sets]]
```

For example,

```
CaseToSupport[l[c[1], -c[1]]] = GenerateTuples[{nz, -nz}]
```

```
{{-Fl2, -Fl1}, {-Fl1, -Fl2}}
```

We compute the fifth partial wave invariant using the result from this notebook (and not the manually reduced result of Theorem 5.8). For this we need to compute the following three cases.

```
CaseToSupport[l[c[1], -c[1], c[1], -c[1]]] :=
 GenerateTuples[{nz, -nz, nz, -nz}]
CaseToSupport[l[c[1], -c[1], c[3], -c[3]]] :=
 GenerateTuples[{nz, -nz, -nz, nz}]
CaseToSupport[l[c[1], c[2], -c[2], -c[1]]] :=
 GenerateTuples[{nz, nz, -nz, -nz}]
```

These sets can be used to compute the partial wave invariants explicitly for the kind of potentials assumed here.

```
ApplyQtoSumQ[exp_Plus] := ApplyQtoSumQ /@ exp
ApplyQtoSumQ[SumQ[case_, exp_]] :=
 Plus @@ (ApplyQtoSummand[exp] /@ (CaseToSupport@case))
ApplyQtoSummand[exp_][tuple_] :=
 (Times @@ Q /@ tuple) *
  (exp /. {Trct[i_, j_] :> Trct[tuple[[i]] * tuple[[j]]],
      ct[i_, l] :> SignFl[tuple[[i]], l], ct[i_] :> tuple[[i]]} /.
    Trct[-cd_] → -Trct[cd])
```

Here, `SignFl` takes care of the minus signs when applying the dual lattice vectors to `l`.

```
SignFl[c_, l_] := c[l]
SignFl[-c_, l_] := -c[l]
```

The fourth partial wave invariant evaluates as follows.

```
ApplyQtoSumQ[SumQ[l[c[1], -c[1]],
    48 Ft[1, ct[1], ct[2]] / ct[1, l]^3]] /.
 {Fl2[l] → -Fl1[l], Ft[1, -Fl1, -Fl2] → Ft[1, Fl1, Fl2],
  Ft[1, -Fl2, -Fl1] → -Ft[1, Fl1, Fl2]}
```

$$-\frac{96\,\text{Ft}[1,\text{Fl1},\text{Fl2}]\,Q[-\text{Fl1}]\,Q[-\text{Fl2}]}{\text{Fl1}[l]^3}$$

To compute the fifth partial wave invariant we first remove the Q-sums with trivial cases. Then we compute the remaining terms for the given potential and after that we apply the assumption that `Trct[Fl1 Fl2]` and `Ft[1,Fl1,Fl2]` vanish.

```
Expand[
 ApplyQtoSumQ[
    wi[5] /.
     {QmFl → 0, SumQ[case_ /; ContainsQ[case, 0 | Plus], _] →
       0}] /. {Fl2[l] → -Fl1[l],
    Ft[i_, -Fl1, -Fl2] → Ft[i, Fl1, Fl2],
    Ft[i_, -Fl2, -Fl1] → (-1)^i Ft[i, Fl1, Fl2]} /.
  {Trct[Fl1 Fl2] → 0, Ft[1, Fl1, Fl2] → 0}]
```

$$\frac{960\,\text{Ft}[2,\text{Fl1},\text{Fl2}]\,Q[-\text{Fl1}]\,Q[-\text{Fl2}]}{\text{Fl1}[l]^4}$$

5.3 Correctness

Let us close this notebook with some considerations on the correctness of the computations performed here. Is there a way to check the correctness of the computations at least heuristically? One way to do so is to use the necessary conditions of Section 4.6. In the computations of the wave invariants above we have used those conditions to decrease the memory requirements and increase the speed of the computations. But alternatively we can choose not to use those conditions in the computation and to then test whether they are satisfied in the end. To this end we set

```
SetSpeed[Thorough]
```

We consider two exemplary cases: Let us first use `Unset` to remove previously memoized results.

```
WD[3, Large] =.
WI[4, 4] =.
```

In the `Thorough` mode the computation of the third partial wave invariant in `Large` dimensions takes around ten seconds instead of one. But as we can see it is still free of `at`, `x` and it vanishes for `Q=0`.

```
FreeQ[WI[3, Large], at]
```

```
True
```

```
FreeQ[WI[3, Large], x]
```

```
True
```

```
WI[3, Large] /. {QmFl → 0, _SumQ → 0}
```

```
0
```

We might ask whether these conditions are trivially true. But this is not the case. Consider the fourth partial wave invariant in dimension `4`, which takes around seven minutes to compute.

```
FreeQ[WI[4, 4], at]
```

```
False
```

```
FreeQ[WI[4, 4], x]
```

```
False
```

```
ByteCount[WI[4, 4] /. {QmFl → 0, _SumQ → 0}]
```

```
22 055 056
```

In this case neither of the necessary conditions is obviously satisfied and one might conclude that this result is incorrect. This is not the case. If we replace the Einstein summations over `Wi`-variables by explicit sums over `W1`, `W2` and `W3` using `ReplaceAllWi` we obtain an expression that again satisfies the necessary conditions from Section 4.6.

```
EX = ReplaceAllWi[WI[4, 4]];
```

```
FreeQ[EX, at] && FreeQ[EX, x]
```

```
True
```

```
EX /. {QmFl → 0, _SumQ → 0}
```

```
0
```

5.4 Technicalities

At the end of this notebook we include some minor technicalities. First, we do not want *Mathematica* to abort the calculation of invariants because the number of nested functions exeeds the `$RecursionLimit`. This limit can be removed by setting it to `Infinity`.

```
$RecursionLimit = Infinity;
```

Also, the following function could be taken from the *Combinatorica* package and is only defined here to avoid loading this package. The function defined here is slightly slower but this is irrelevant for the small n used here.

`Partitions[n]`
returns a `List` of all partitions of the number n.

```
Partitions[n_] := Partitions[n, n]

Partitions[0, _] := Sequence[]
Partitions[n_, max_] :=
 (Sequence @@
     Flatten /@ Distribute[{#, Partitions[n - #, #]}, List]) & /@
  Range[Min[n, max], 1, -1]
```

We also need a function to test whether one list is a subset of another. This function is included in *Mathematica* version 10 and higher.

```
If[$VersionNumber < 10,
 SubsetQ[list1_, list2_] := Complement[list2, list1] === {}
]
```

`SubsetQ` gives `True` exactly if *list2* is a subset of *list1*.

Custom Tree Form

Some complex expressions are easier to understand if they are represented in the form of a graph. While *Mathematica* contains a function `TreeForm`, which returns a tree representation of some given expression, it will be more convenient to use a custom version of this function.

`CTreeForm[exp]`
displays a tree representing *exp* following the conventions used in Section B.3.

This function is not critical to the computation of wave invariants and thus there is no need for a detailed explanation.

Implementation

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Notation

ω	nondegenerate, Hermitian line bundle
$\omega(z)$	Morse coordinates, Lemma 4.18 and Appendix A
$v(z)$	volume form of Morse coordinates $\omega(z)$
a	$a \in \mathbb{R}^{n\prime}$, also denotes the connection $\nabla^{\mathrm{D}} + \tilde{a}$, 1.24
A_x^{D}	$-\tilde{w}_x$
A_x	$A_x^{\mathrm{D}} + \tilde{a}$
$r_1 \mid \cdots \mid r_m$	Chern invariant factors
F	nondegenerate, bilinear map $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ or $\mathbb{R}^n \to \mathbb{R}^{n\prime}$
$\tilde{a}, \tilde{c}, \tilde{F}$	factor $2\pi\mathrm{i}$, $\tilde{a} \coloneqq 2\pi\mathrm{i} \cdot a$, $\tilde{F}_k = (\tilde{F})_k = (2\pi\mathrm{i})^k F_k$
F_k	curvature trace, 3.7
$\langle f, g \rangle$	$\frac{1}{\operatorname{Vol} M} \int_M f \cdot \overline{g} \, \mathrm{d}V$
E_c	$E_c = \mathrm{e}^{-\tilde{c}}$
Q_c	$\langle Q, E_c \rangle$
$\overset{\tau}{=}$	equal up to τ-integration, Notation 4.26
$\to_i$	substitution of variables, Notation 4.27
$\overset{a_0}{=}$	equal up to factors of a_0, Notation 4.28
$\overset{\mathrm{NC}}{=}$	equal up to necessary conditions, Notation 4.43
$\overset{x}{=}$	equal up to x-integration, Notation 4.44
$\cong$	equal up to a combination of other notations
$H(i, j, k)$	Section 4.4
$\mathcal{L}'$	dual lattice
$\mathcal{L}'_Q$	frequency support, $\{c \in \mathcal{L}' \mid Q_c \neq 0\}$
$\mathcal{L}_Q$	lattice support, $\{l \in \mathcal{L} \mid Q_{Fl} \neq 0\}$
W_i	$\{W_1, \ldots, W_{n-1}, l/\lvert l \rvert\}$ orthonormal basis
$\sum^Q$	Q-sum, 5.5
$l[\ldots]$	case, 5.1